Coincidences and Colorings of Lattices and $\mathbb{Z}$-modules

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Dissertation zur Erlangung des Doktorgrades
an der
Fakultät für Mathematik
Universität Bielefeld

vorgelegt von

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Universität Bielefeld

November 2010

1. Berichterstatter: Prof. Dr. Michael Baake und Dr. Peter Zeiner
2. Berichterstatter: Prof. Dr. Uwe Grimm

Datum der mündlichen Prüfung: 25. Januar 2011

Prüfungsausschuss: Prof. Dr. M. Baake, Prof. Dr. W.-J. Beyn, Prof. Dr. H. Krause, Prof. Dr. M. Kaßmann, Dr. P. Zeiner

Gedruckt auf alterungsbeständigem Papier °°ISO 9706

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Acknowledgements

I would like to express my deepest gratitude to the following people and institutions who made this work (directly or indirectly) possible:

To *Prof. Dr. Michael Baake*, for giving me the opportunity to work in his research group, and for his support, guidance, and encouragement during my entire stay in Bielefeld.

To *Dr. Peter Zeiner*, for sharing his knowledge and expertise, for the helpful and valuable discussions, and for his input and thoroughness in reviewing drafts of this thesis.

To my second reviewer, *Prof. Dr. Uwe Grimm*, and to the other members of my doctoral committee; *Prof. Dr. Wolf-Jürgen Beyn*, *Prof. Dr. Henning Krause*, and *Prof. Dr. Moritz Kaßmann*, for taking time out of their busy schedules to read my work.

To the *German Academic Exchange Service* (DAAD), the *Research Center for Mathematical Modeling* (FSPM) at the University of Bielefeld, and the *Collaborative Research Center (CRC) 701: "Spectral Structures and Topological Methods in Mathematics"*, for financial support of my doctoral studies.

To the *Institute of Mathematics* at the University of the Philippines (UP), Diliman, for granting me leave of absence to pursue my doctoral studies.

To present and former members of the research group "*Mathematik in den Naturwissenschaften*"; Michael Baake, Christoph Richard, Franz Gähler, Peter Zeiner, Dirk Frettlöh, Christian Huck, Johan Nilsson, Uwe Schwerdtfeger, Manuela Heuer, Svenja Glied, Kai Miguel Matzutt, Natascha Neumärker, Markus Moll, Enrico Paolo Bugarin, Claudia Lütkehölter, Oliver Schmidt, Nadine Eisner, Magnus Dümke, and Thomas Blomenkamp, for providing a stimulating and friendly work atmosphere, and for interesting and funny discussions during lunch.

To my family here in Germany, the *Bayanihan Pilipino e.V.*, in particular, Kuya Filemon, German, Larry, and Ate Babes, Becca, Cris, Edna, Flor, Glecy, Grace, Larife, Linda, Lisa, Lita, Lulu, Marissa, Nancy, Rosie, Yeny; as well as Ate Belinda, Josie, Chit, Virgie, and Judith.

To my fellow Filipino students here in Germany; *Andrew*, *Bugs*, *Gail*, *Gori*, *Karl*, *Migs*, and *Santi*, for the friendship, dinners, and quiz nights.

To the *International Office* at the University of Bielefeld for making the life of international students like me a little bit easier and more fun.

To all acquaintances and friends I met in my German language classes in Bielefeld and in Marburg, and in the excursion to Brussels.

To my fellow doctoral students: *Gino*, *Carmen*, *Romar*, *Tina*, and *Bituin*, for visiting me in Bielefeld, the travels in Europe, and many chat sessions.

To all my former mathematics teachers, for sharing your knowledge with me.

To all my friends, for all the things that you have done for me and for believing in me.

To my family, *Daddy*, *Mommy*, *Joyce*, and *Jandriel*, for always being there for me. I love you all.

Finally, to the **Almighty God**, for the blessings you have given me all these years despite my weaknesses and shortcomings.

Introduction

Background

It was Friedel in 1911 who first recognized the usefulness of coincidence site lattices (CSLs) in describing and classifying grain boundaries of crystals [**25**]. Since then, CSLs have been an indispensable tool in the study of grain boundaries, twins, and interfaces [**50, 15, 14, 76, 61**]. This prompted various authors to examine the CSLs of specific lattices, for instance, cubic and hexagonal crystals [**65, 39, 33, 34, 35, 37, 40**].

The advent of quasicrystals in 1984 triggered a renewed interest in CSLs. This is because experimental evidence showed that quasicrystals, like ordinary crystals, exhibit multiple grains, twin relationships, and coincidence quasilattices [**75, 77, 63, 79**]. A need for a more general and mathematical treatment of the coincidence problem ensued, and this was dealt with in [**4**]. Known results for lattices were again considered and reformulated so that they may be readily extended to aperiodic situations. This was necessary since the first stage in solving the coincidence problem for quasicrystals involves calculating the coincidence site modules (CSMs) of the underlying translation modules, such as modules with 5, 8, 10, and 12-fold symmetry (see [**59, 4**] and references therein, see also [**62**]). Of equal mathematical interest are the sets of (linear) coincidence isometries of a lattice or module, since these sets form a subgroup of the orthogonal group and they contain the point symmetry group of the lattice or module, respectively.

Today, many results are known about the coincidences of lattices and modules in dimensions $d \leq 4$. The coincidence problem for certain planar lattices and modules was solved in [**59, 4**] using factorization properties of cyclotomic integers. For lattices and modules in dimensions three and four, quaternions have proven to be an appropriate tool. Results on the coincidences of three-dimensional cubic lattices and modules can be found in [**4, 81, 10**], while the coincidences of four-dimensional lattices and modules were investigated in [**78, 68, 4, 82, 13, 7, 44, 45**].

Several authors also considered the CSL problem from a different perspective. In [**23, 24, 21**], a matrix theory for CSLs was developed via factorizations of rational and integer matrices. Based on these results, a formula for the coincidence indices of certain coincidence isometries of the hypercubic lattice $\mathbb{Z}^d$ was derived [**87**]. In addition, the decomposition of coincidence isometries of lattices and modules in Euclidean d-space as a product of at most d coincidence reflections was considered in [**88, 47**]. Another approach to the coincidence problem for lattices using geometric algebra was established in [**67, 2**].

Connections of the coincidence problem for lattices and modules to other related topics have also been explored. The relationship between the sets of coincidence and similarity isometries of lattices and modules were examined in [**30, 28, 29**]. Also, in [**29**], the generalized dihedral subgroups of the set of coincidence rotations of the cubic lattices and the standard icosahedral modules were considered. On the other hand, an extension of CSLs to multiple coincidence site lattices (MCSLs) has been carried out in [**6, 12, 84**]. Interest in MCSLs has been motivated not only by the study of triple junctions and quadruple points, and more generally, multiple junctions of grains, and other multicrystal assemblies [**26**], but also by the problem of optimal lattice quantizers in [**72**] wherein a lattice is expressed as the intersection of simpler lattices.

Similar to CSLs, a revived interest on color symmetries of (quasi)crystals and tilings in recent years was brought upon by the discovery of quasicrystals, see [**58, 51, 3, 8, 9, 5, 19, 54, 55, 16**]. Despite being two different problems, the enumeration and classification of color symmetries of lattices come hand in hand with the identification of CSLs [**69, 70, 59, 3, 54, 55**].

Outline of the thesis

The first chapter gives all the essential definitions, notations, and results for this thesis. It starts with a discussion of the coincidence problem for an arbitrary lattice or $\mathbb{Z}$-module. A summary of the results on the coincidences of the square lattice, some n-planar modules, cubic lattices, and hypercubic lattices follows the general treatment. Notions on colorings of lattices and $\mathbb{Z}$-modules end the chapter.

It is well-known that a lattice and its sublattices have the same set of coincidence isometries. In fact, not only are the coincidence isometries for the three cubic lattices the same, but also are the coincidence indices for a given coincidence isometry. This is due to a particular shell structure of the lattice points: points at the corners of a cube and those in the center or on the faces of the cube lie on different shells, and thus cannot be mapped onto each other by an isometry [**39**]. On the other hand, aside from having different point groups, the two four-dimensional hypercubic lattices do not share the same set of coincidence indices (the coincidence indices of the centered type are all odd while those of the primitive type are odd or twice an odd number) [**4, 82**]. This motivates the following questions: Under which conditions does a sublattice have the same coincidence indices as the lattice itself? Is it possible to calculate the coincidence indices of a sublattice once the coincidence indices of its parent lattice are already known? Chapter 2 gives some answers to these questions by looking at certain colorings of lattices.

A method of computing the coincidence index of a coincidence isometry of a lattice with respect to a sublattice is formulated in Theorem 2.4 via properties of the coloring of the lattice determined by the sublattice. This result motivates a generalization of the idea of color symmetry to that of a color coincidence. Theorem 2.8 shows that the color coincidences of a coloring of a lattice induced by some sublattice are precisely those coincidence isometries of the lattice that fix the sublattice. This allows an association between the property of being a color coincidence and the relationship between the coincidence indices with respect to the lattice and to its sublattice. In particular, if R is a coincidence isometry that is a color coincidence of the coloring of the lattice (induced by a sublattice), then the coincidence index of R with respect to the lattice is divisible by the coincidence index of R with respect to the sublattice (Corollary 2.10). Attention is also given to the set formed by the color coincidences of a coloring of a lattice. Examples, including one involving the set of vertices of the Ammann-Beenker tiling, and other general results are provided to illustrate these ideas.

The mathematical treatment of the coincidence problem is very often restricted to linear coincidence isometries, that is, rotations and improper rotations, whereas isometries containing a translational part are ignored. Nevertheless, general (affine) isometries are important in crystallography. Indeed, the situation where one shifts the two component crystals against each other has been investigated in [**27, 22**] and references therein. It was shown that these shifts are needed to minimize the grain boundary energy, thus they are often referred to as "rigid relaxations". However, some authors claim that minimizing the energy may require shifts that destroy all coincidence sites.

Even though the idea of introducing a shift after applying a linear coincidence isometry has already been dealt with in the physical literature, not much can be found in the mathematical literature where a systematic treatment of the subject is still missing. Some steps in this general direction have actually been made in the appendix of [**59**]. There, the authors considered coincidence isometries about certain points which are not lattice or module points. For instance, they determined the set of coincidence isometries about the center of a Delauney cell of the square lattice and calculated the corresponding indices.

In Chapter 3.1, the notion of a CSL and CSM is extended to intersections of two lattices and $\mathbb{Z}$-modules, respectively, that are related by any isometry. Such intersections are referred to as affine coincidence site lattices/modules (ACSLs/ACSMs), and the isometries that generate these intersections as affine coincidence isometries. Theorem 3.3 identifies the affine coincidence isometries of a lattice or $\mathbb{Z}$-module, while (3.1) gives the resulting intersection. In the event that the set of affine coincidence isometries of a lattice or $\mathbb{Z}$-module forms a group, then it must be the symmetry group of the lattice or $\mathbb{Z}$-module.

The rest of Chapter 3 covers a related and special case: the coincidence problem for shifted lattices and shifted $\mathbb{Z}$-modules. That is, after translating the lattice or $\mathbb{Z}$-module Γ by some vector x, and upon application of a linear isometry R to the shifted lattice or shifted $\mathbb{Z}$-module $x+\Gamma$ (with respect to the origin), its intersection with $x+\Gamma$ is considered. Equation (3.2) states that the said operation corresponds to shifting the intersection of Γ with the image of Γ under the affine isometry $(Rx-x, R)$ by x. Note that the effect of the affine isometry (Rx, R) on Γ is equivalent to applying the linear isometry R on Γ about a different point $(-x)$, thus keeping at least one point $(-x)$ fixed. Theorem 3.8 asserts that the (linear) coincidence isometries of $x+\Gamma$ are those coincidence isometries R of Γ that satisfy $Rx - x \in \Gamma + R\Gamma$. Moreover, the CSLs/CSMs of the shifted lattice/$\mathbb{Z}$-module are merely translates of CSLs/CSMs of the original lattice/$\mathbb{Z}$-module. Hence, no new values of coincidence indices are obtained by shifting the lattice, with some values disappearing or their multiplicity changed.

Similar to the approach in [**59, 4**], an extensive analysis of the coincidences of a shifted square lattice in Chapter 3.4 is achieved by identifying the lattice with the ring of Gaussian integers. The coincidence problem is completely solved when the shift consists of an irrational component (Theorem 3.26). For the remaining case, that is, when the shift may be written as a quotient of two Gaussian integers that are relatively prime, one computes for the set of coincidence rotations of the shifted square lattice using some divisibility condition involving the denominator of the shift (Lemma 3.28). In both instances, the set of coincidence rotations of a shifted square lattice form a group. An example is given where the set of coincidence isometries of a shifted square lattice is not a group. This shows that in general, the set of coincidence isometries of a shifted lattice does not form a group. Corresponding results and an example for planar modules conclude the chapter.

The final chapter of this thesis is concerned with the coincidences of sets of points formed by the union of a lattice with a finite number of shifted copies of the lattice. Such sets are referred to as multilattices. This idea should be useful in the context of bicrystallography, and in general, to crystals having multiple atoms per primitive unit cell [**31, 60**]. The chapter starts with an analysis of the coincidences of the simplest multilattice, that is, of the union of a lattice and a shifted lattice. This leads to the solution of the coincidence problem for the diamond packing given in Theorem 4.6. The main result of the chapter is Theorem 4.15, which gives the solution of the coincidence problem for general multilattices. Simply put, the (linear) coincidence isometries of a multilattice are exactly the coincidence isometries of the lattice that generates the multilattice - only the resulting intersections and corresponding indices may vary.

The main problem in Chapter 2 is then revisited, where the reverse condition is now considered. More accurately, if the coincidence problem for a sublattice of a given lattice has already been solved, then what can be deduced about the CSLs and corresponding coincidence indices of the original lattice? This question is resolved in Theorem 4.17 by regarding the lattice as a multilattice formed by the union of the sublattice with the cosets of the sublattice. This perspective establishes a connection among the relationship between the coincidence indices of a lattice and a sublattice, color coincidences of the coloring of the lattice determined by the sublattice, and coincidences of shifted lattices, which is encapsulated in Propositions 4.19 and 4.20. The chapter ends with a full description of the case when a sublattice is of prime index in a lattice, and the solution of the coincidence problem for certain primitive and centered rectangular lattices.

CHAPTER 1

Preliminaries

Let us recall the necessary background and results for this thesis first.

1.1. Coincidences of lattices and $\mathbb{Z}$-modules

We start with the basic definitions and general results on coincidence isometries of lattices and $\mathbb{Z}$-modules. A detailed discussion of these can be found in [**4, 83**].

A discrete subset Γ of $\mathbb{R}^d$ is a *lattice* (of *rank* and *dimension* d) if it is the $\mathbb{Z}$-span of d linearly independent vectors $v_1, \ldots, v_d \in \mathbb{R}^d$ over $\mathbb{R}$. The set $\{v_1, \ldots, v_d\}$ is called a *basis* of Γ, and $\Gamma = \mathbb{Z}v_1 \oplus \ldots \oplus \mathbb{Z}v_d$. As a group, Γ is isomorphic to the free abelian group of rank d. Alternatively, one can characterize a lattice as a discrete co-compact subgroup of $\mathbb{R}^d$.

A subset Γ' of the lattice Γ is a *sublattice* of Γ if Γ' is a subgroup of Γ of finite index, that is, if $[\Gamma : \Gamma'] < \infty$. Hence, Γ' is itself a lattice and is of the same rank and dimension as Γ. Here, the index of Γ' in Γ may also be interpreted geometrically – $[\Gamma : \Gamma']$ is the quotient of the volume of a fundamental domain of Γ' by the volume of a fundamental domain of Γ.

The *dual* of a lattice Γ in $\mathbb{R}^d$ is the lattice

$$\Gamma^* := \left\{x \in \mathbb{R}^d : \langle x, y\rangle \in \mathbb{Z} \text{ for all } y \in \Gamma\right\},$$

where $\langle \cdot, \cdot \rangle$ denotes the standard scalar product in $\mathbb{R}^d$. If $B = \{v_1, \ldots, v_d\}$ is a basis for Γ, then $\{v_1^*, \ldots, v_d^*\}$, where $\left\langle v_j^*, v_k\right\rangle = \delta_{j,k}$ for $0 \leq j, k \leq d$, is a basis for Γ^* and is referred to as a *dual basis* for B. Given a sublattice Γ' of Γ, Γ^* is a sublattice of $(\Gamma')^*$ with $[(\Gamma')^* : \Gamma^*] = [\Gamma : \Gamma']$ and $(\Gamma')^*/\Gamma^* \cong \Gamma/\Gamma'$.

Two lattices Γ_1 and Γ_2 are said to be *commensurate*, denoted $\Gamma_1 \sim \Gamma_2$, if $\Gamma_1 \cap \Gamma_2$ is a sublattice of both Γ_1 and Γ_2. Commensurateness between lattices defines an equivalence relation. Given two commensurate lattices Γ_1 and Γ_2, their *sum*

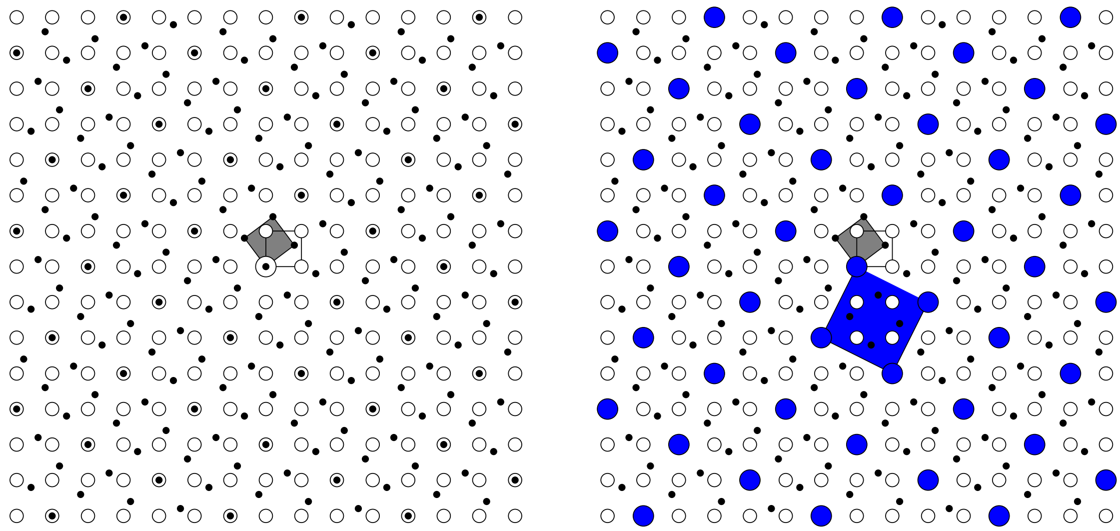
$$\Gamma_1 + \Gamma_2 := \{x_1 + x_2 : x_1 \in \Gamma_1, x_2 \in \Gamma_2\}$$

is also a lattice and the following equations are true: $(\Gamma_1 \cap \Gamma_2)^* = \Gamma_1^* + \Gamma_2^*$ and $(\Gamma_1 + \Gamma_2)^* = \Gamma_1^* \cap \Gamma_2^*$.

An orthogonal transformation $R \in O(d) := O(d, \mathbb{R})$ is a (*linear*) *coincidence isometry* of the lattice Γ in $\mathbb{R}^d$ if $\Gamma \sim R\Gamma$. The sublattice $\Gamma(R) := \Gamma \cap R\Gamma$ is called the *coincidence site lattice* (CSL) of Γ generated by R, while the index of $\Gamma(R)$ in Γ, $\Sigma_\Gamma(R) := [\Gamma : \Gamma(R)] = [R\Gamma : \Gamma(R)]$, is called the *coincidence index of R with respect to* Γ. Geometrically, $\Sigma_\Gamma(R)$ gives the ratio of the volume of a fundamental domain of the CSL $\Gamma(R)$ with the volume of a fundamental domain of Γ or of $R\Gamma$. If no confusion arises, we simply write $\Sigma(R)$ to denote the coincidence index of R. Clearly, symmetries in the point group of Γ, $P(\Gamma) = \{R \in O(d) : R\Gamma = \Gamma\}$, are precisely those coincidence isometries R of Γ with $\Sigma(R) = 1$.

The set of (linear) coincidence isometries of a lattice Γ is denoted by $OC(\Gamma)$ while the set of coincidence rotations of Γ, that is, $OC(\Gamma) \cap SO(d)$, is written as $SOC(\Gamma)$. Since commensurateness of lattices is an equivalence relation, the set $OC(\Gamma)$ forms a group having $SOC(\Gamma)$ as a subgroup.

Example 1.1: Consider the square lattice $\Gamma = \mathbb{Z}^2$. Let $R \in O(2)$ be the rotation about the origin by $\theta = \tan^{-1}(\frac{3}{4})$ in the counterclockwise direction. Figure 1(a) shows points on the lattice Γ (white dots) and on the rotated copy of Γ, $R\Gamma$ (black dots). One also sees a fundamental domain for Γ (white square) and for $R\Gamma$ (gray square), both having the same volume. The points where the white dots and the black dots coincide correspond to points in $\Gamma \cap R\Gamma$. Since the points of intersection of Γ and $R\Gamma$ form a sublattice of Γ (and $R\Gamma$), R is a coincidence rotation of Γ. The CSL generated by R is precisely these points of intersection, shown in Figure 1(b) as the lattice formed by the blue dots. Figure 1(b) also shows a fundamental domain of $\Gamma(R)$ (blue square) which is five times larger than that of the fundamental domains of Γ and $R\Gamma$. This indicates that $\Gamma(R)$ is of index 5 in Γ (and $R\Gamma$), and so $\Sigma(R) = 5$.



(a) lattices Γ and $R\Gamma$ (b) CSL $\Gamma(R)$ with $\Sigma(R) = 5$

Figure 1. The lattices Γ (white dots), $R\Gamma$ (black dots), and $\Gamma(R)$ (blue dots), where $\Gamma = \mathbb{Z}^2$ and $R \in OC(\Gamma)$ is the counterclockwise rotation about the origin by $\theta = \tan^{-1}(\frac{3}{4}) \approx 37^{\cdot}$. The white, gray, and blue squares correspond to fundamental domains for Γ, $R\Gamma$, and $\Gamma(R)$, respectively. The origin is the common vertex of the fundamental domains.

The following are immediate.

Proposition 1.2: *Let $\Gamma \subseteq \mathbb{R}^d$ be a lattice and $R \in OC(\Gamma)$. Then $R^{-1} \in OC(\Gamma)$ with $\Sigma(R^{-1}) = \Sigma(R)$ and $R[\Gamma(R^{-1})] = \Gamma(R)$.*

Theorem 1.3: *Let Γ be a lattice in $\mathbb{R}^d$.*

(i) *If $\lambda \in \mathbb{R}^+$ then $OC(\lambda\Gamma) = OC(\Gamma)$ with $\Sigma_{\lambda\Gamma}(R) = \Sigma_\Gamma(R)$ for all $R \in OC(\lambda\Gamma)$.*

(ii) *If $S \in O(d)$ then $OC(S\Gamma) = S[OC(\Gamma)]S^{-1} = \{SRS^{-1} : R \in OC(\Gamma)\} \cong OC(\Gamma)$ with $\Sigma_{S\Gamma}(R) = \Sigma_\Gamma(S^{-1}RS)$ for all $R \in OC(S\Gamma)$.*

Theorem 1.3 implies that the groups of coincidence isometries of similar lattices are conjugate subgroups of $O(d)$. Moreover, corresponding coincidence isometries (under conjugation) of similar lattices have equal coincidence indices.

The next theorem shows that dual lattices share the same group of coincidence isometries and the same set of coincidence indices.

Theorem 1.4: *Let $\Gamma \subseteq \mathbb{R}^d$ be a lattice. Then $OC(\Gamma) = OC(\Gamma^*)$ and $\Sigma_\Gamma(R) = \Sigma_{\Gamma^*}(R)$ for all $R \in OC(\Gamma)$.*

Theorem 1.5: *Let Γ_2 be a sublattice of the lattice Γ_1 in $\mathbb{R}^d$. Then $OC(\Gamma_1) = OC(\Gamma_2)$.*

Remark 1.6: Given an $R \in OC(\Gamma_1) = OC(\Gamma_2)$, we shall denote by $\Sigma_1(R)$ and $\Sigma_2(R)$ the coincidence indices of R with respect to Γ_1 and Γ_2, respectively.

Even though the groups of coincidence isometries of a lattice and sublattice are the same, the coincidence indices and corresponding multiplicities with respect to the two lattices are in general different. The following proposition states the known result on this issue.

Proposition 1.7: *Let Γ_1 be a lattice in $\mathbb{R}^d$, Γ_2 be a sublattice of Γ_1 of index m, and $R \in OC(\Gamma_1)$. Then $\Sigma_1(R) \mid m\,\Sigma_2(R)$.*

Remark 1.8: Suppose Γ_2 is a sublattice of Γ_1 in $\mathbb{R}^d$ of index m. Since Γ_1^* is a sublattice of Γ_2^*, it follows from Proposition 1.7 and Theorem 1.4 that $\Sigma_2(R) \mid m\,\Sigma_1(R)$ for all $R \in OC(\Gamma_1)$.

The following result about the coincidence index of the product of two coincidence isometries can be found in [**7, 86**].

Proposition 1.9: *Let $\Gamma \subseteq \mathbb{R}^d$ be a lattice and R_1, $R_2 \in OC(\Gamma)$.*

(i) *Then $\Sigma(R_2R_1)$ divides $\Sigma(R_2) \cdot \Sigma(R_1)$.*

(ii) *If $\Sigma(R_1)$ and $\Sigma(R_2)$ are relatively prime, then $\Sigma(R_2R_1) = \Sigma(R_2) \cdot \Sigma(R_1)$, $\Gamma(R_2R_1) = \Gamma \cap R_2\Gamma \cap R_2R_1\Gamma$, and $R_2\Gamma = \Gamma(R_2) + R_2\Gamma(R_1)$.*

In the quasicrystallographic setting, it is necessary to consider the coincidence problem for certain $\mathbb{Z}$-modules in $\mathbb{R}^d$. If r linearly independent vectors over $\mathbb{Z}$ span $\mathbb{R}^d$ over $\mathbb{R}$, then the subset $\mathcal{M}$ of $\mathbb{R}^d$ spanned by these r vectors over $\mathbb{Z}$ is called a *$\mathbb{Z}$-module* (of *rank* r and *dimension* d). Since the said r vectors span $\mathbb{R}^d$, $r \geq d$. A module $\mathcal{M}$ of rank r and dimension d that is discrete (and hence, $r = d$) is a lattice.

Remark 1.10: A $\mathbb{Z}$-module of rank r and dimension d forms a group that is isomorphic to the free abelian group of rank r. This means that as a group, a $\mathbb{Z}$-module can be thought of as a lattice in $\mathbb{R}^r$. Therefore, results for lattices that were obtained using only properties of lattices as a group must also hold for $\mathbb{Z}$-modules.

Hence, the notions of *submodule*, *commensurateness*, and that of a (*linear*) *coincidence isometry* are well-defined and are defined analogously as in the lattice case. In this instance, the set of coinciding points forms a submodule and is thus called a *coincidence site module* (CSM). However, a bit more care is needed in defining the coincidence index of a coincidence isometry R of a $\mathbb{Z}$-module $\mathcal{M}$. It is assumed throughout this thesis that if $\mathcal{M}(R) := \mathcal{M} \cap R\mathcal{M}$ then $[\mathcal{M} : \mathcal{M}(R)] = [R\mathcal{M} : \mathcal{M}(R)]$. This value is then defined as the *coincidence index of R with respect to $\mathcal{M}$*, denoted by $\Sigma_{\mathcal{M}}(R)$ or simply $\Sigma(R)$. This requirement is easily satisfied by lattices in $\mathbb{R}^d$, but is not trivial for $\mathbb{Z}$-modules [**85**]. Nonetheless, the said requirement is equivalent to $\Sigma(R) = \Sigma(R^{-1})$, a condition satisfied by, among others, certain planar n-modules (see Subsection 1.2.2). Furthermore, in general, the dual of a $\mathbb{Z}$-module is not defined.

Since the results above for lattices (except for Theorem 1.4 and Remark 1.8, because they involve the dual lattice) were obtained via some group-subgroup relationship, corresponding results for $\mathbb{Z}$-modules are also true.

1.2. Solution of the coincidence problem for certain lattices and $\mathbb{Z}$-modules

Results on coincidence isometries and CSLs of the square, cubic, and hypercubic lattices shall be discussed in this section. The coincidence problem for certain $\mathbb{Z}$-modules of cyclotomic integers is also examined.

1.2.1. Square lattice. Let us look at the square lattice $\mathbb{Z}^2$ first (see [**4, 59**] for details). Since $O(2)$ is the semidirect product of $SO(2)$ and the cyclic group C_2 generated by the reflection in the x-axis, the discussion is restricted to coincidence rotations at the outset and later on extended to coincidence reflections.

The group of coincidence rotations of $\mathbb{Z}^2$ is $SOC(\mathbb{Z}^2) = SO(2, \mathbb{Q})$. To determine the structure of this group, the square lattice is identified with the ring of Gaussian integers $\Gamma = \mathbb{Z}[i] = \left\{m + ni : m, n \in \mathbb{Z}, i = \sqrt{-1}\right\}$, embedded in the set of complex numbers $\mathbb{C}$. In this setting, every rotation in $SO(2)$ by an angle of θ in the counterclockwise direction corresponds to multiplication by the complex number $e^{i\theta}$ on the unit circle. Because the ring $\mathbb{Z}[i]$ is a Euclidean domain and thus a unique factorization domain (see [**43**]), a coincidence rotation R of Γ is equivalent to multiplication by a complex number

$$\varepsilon \cdot \prod_{p \equiv 1(4)} \left(\frac{\omega_p}{\overline{\omega_p}}\right)^{n_p}, \tag{1.1}$$

where $n_p \in \mathbb{Z}$ and only a finite number of $n_p \neq 0$, ε is a unit in $\mathbb{Z}[i]$, p runs over the splitting primes in $\mathbb{Z}[i]$, that is, rational primes $p \equiv 1 \pmod 4$, and ω_p, and its complex conjugate $\overline{\omega_p}$, are the Gaussian prime factors of $p = \omega_p \cdot \overline{\omega_p}$. If one denotes by z the numerator of (1.1), that is,

$$z = \prod_{\substack{p \equiv 1(4) \\ n_p > 0}} {\omega_p}^{n_p} \cdot \prod_{\substack{p \equiv 1(4) \\ n_p < 0}} \left(\overline{\omega_p}\right)^{-n_p}, \tag{1.2}$$

then the coincidence index of R is equal to the number theoretic norm of z, $\Sigma(R) = N(z) := z \cdot \overline{z} = |z|^2$. In addition, the CSL obtained from R is the principal ideal

$\Gamma(R) = (z) := z\mathbb{Z}[i]$. Consequently, the group of coincidence rotations of the square lattice is given by $SOC(\mathbb{Z}^2) = SO(2,\mathbb{Q}) \cong C_4 \times \mathbb{Z}^{(\aleph_0)}$, where C_4 is the cyclic group of order 4 generated by i, and $\mathbb{Z}^{(\aleph_0)}$ is the direct sum of countably many infinite cyclic groups each of which is generated by $\frac{\omega_p}{\overline{\omega_p}}$.

Every coincidence reflection $T \in OC(\Gamma) \setminus SOC(\Gamma)$ can be written as $T = R \cdot T_r$, where $R \in SOC(\Gamma)$ and T_r is the reflection along the real axis (corresponding to complex conjugation). Since T_r leaves Γ invariant, $\Sigma(T) = \Sigma(R)$ and $\Gamma(T) = \Gamma(R)$. Finally, one obtains that $OC(\mathbb{Z}^2) = O(2,\mathbb{Q}) = SOC(\mathbb{Z}^2) \rtimes \langle T_r \rangle$ (where $\rtimes$ stands for semidirect product).

The coincidence indices and the number of CSLs for a given index m are described by means of a generating function. Let $f_{\mathbb{Z}^2}(m)$ be the number of CSLs of $\mathbb{Z}^2$ of index m. Then $f_{\mathbb{Z}^2}$ is *multiplicative* (that is, $f_{\mathbb{Z}^2}(1) = 1$ and $f_{\mathbb{Z}^2}(mn) = f_{\mathbb{Z}^2}(m)f_{\mathbb{Z}^2}(n)$ whenever m, n are relatively prime), and for primes p and $r \in \mathbb{N}$,

$$f_{\mathbb{Z}^2}(p^r) = \begin{cases} 2, & \text{if } p \equiv 1 \pmod 4 \\ 0, & \text{otherwise.} \end{cases}$$

The generating function for $f_{\mathbb{Z}^2}$ as a Dirichlet series $\Phi_{\mathbb{Z}^2}(s)$ is given by

$$\begin{aligned} \Phi_{\mathbb{Z}^2}(s) &= \sum_{m=1}^{\infty} \frac{f_{\mathbb{Z}^2}(m)}{m^s} = \prod_{p\equiv 1(4)} \left(1 + \frac{2}{p^s} + \frac{2}{p^{2s}} + \ldots\right) = \prod_{p\equiv 1(4)} \frac{1+p^{-s}}{1-p^{-s}} \\ &= 1 + \tfrac{2}{5^s} + \tfrac{2}{13^s} + \tfrac{2}{17^s} + \tfrac{2}{25^s} + \tfrac{2}{29^s} + \tfrac{2}{37^s} + \tfrac{2}{41^s} + \tfrac{2}{53^s} + \tfrac{2}{61^s} \\ &\quad + \tfrac{4}{65^s} + \tfrac{2}{73^s} + \cdots . \end{aligned} \tag{1.3}$$

Observe from (1.3) that the coincidence indices of the square lattice are positive integers all of whose prime factors are splitting primes in $\mathbb{Z}[i]$. The number of coincidence rotations of $\mathbb{Z}^2$ for a given index m is given by $\hat{f}_{\mathbb{Z}^2}(m) = 4f_{\mathbb{Z}^2}(m)$, where the factor 4 stems from the fact that $\mathbb{Z}^2$ has four symmetry rotations. Thus, the Dirichlet series generating function for $\hat{f}_{\mathbb{Z}^2}(m)$ is $4\Phi_{\mathbb{Z}^2}(s)$.

Remark 1.11: Observe from (1.1) and (1.2) that each coincidence rotation R of $\Gamma = \mathbb{Z}^2$ can be associated to a numerator z and unit ε, and this shall be written as $R_{z,\varepsilon}$. Note however that this correspondence is not unique: one can take any associate of z as numerator and the unit ε will change accordingly. Nonetheless, throughout this thesis, $R_{z,\varepsilon} \in SOC(\Gamma)$ stands for multiplication by the complex number $\varepsilon\frac{z}{\overline{z}}$. Here, the fraction $\frac{z}{\overline{z}}$ is assumed to be reduced, that is, z and $\overline{z}$ have no common prime factors. Also, we set $z = 1$ whenever $R_{z,\varepsilon} \in P(\Gamma)$.

Similarly, $T_{z,\varepsilon} \in OC(\Gamma) \setminus SOC(\Gamma)$ shall be understood to be the coincidence reflection $T_{z,\varepsilon} = R_{z,\varepsilon} \cdot T_r$.

1.2.2. Certain planar n-modules. The approach used to solve the coincidence problem for the square lattice can be generalized to certain planar n-modules.

In the complex plane, the standard planar n-module is identified with

$$\mathcal{M}_n = \mathbb{Z} \oplus \mathbb{Z}\xi_n \oplus \mathbb{Z}\xi_n^2 \oplus \ldots \oplus \mathbb{Z}\xi_n^{n-1},$$

where $\xi_n = e^{2\pi i/n}$, an nth root of 1 (see [**56**]). The set $\mathcal{M}_n$ is a $\mathbb{Z}$-module of rank $\phi(n)$ that exhibits N-fold rotational symmetry, where $\phi(n)$ is Euler's totient function and

$N = \mathrm{lcm}(n, 2)$. In fact, $\mathcal{M}_n$ is simply the ring of integers $\mathbb{Z}[\xi_n]$ of the cyclotomic field $\mathbb{Q}(\xi_n)$ [**80**]. Since $\mathcal{M}_{2n} = \mathcal{M}_n$ whenever n is odd, values of n for which $n \equiv 2 \pmod 4$ are excluded. Furthermore, we only consider the cases when $\mathcal{M}_n$ has class number 1, that is, for the following twenty-nine values of n:

$$n = 3, 4, 5, 7, 8, 9, 11, 12, 13, 15, 16, 17, 19, 20, 21, 24,\\ 25, 27, 28, 32, 33, 35, 36, 40, 44, 45, 48, 60, 84.$$

The reason for this is that for these values of n, $\mathcal{M}_n$ is a principal ideal domain, and thus, unique factorization up to units holds.

Let $L := \mathbb{Q}(\xi_n + \xi_n^{-1}) = \mathbb{Q}(\cos\frac{2\pi}{n})$ be the maximal real subfield of $K := \mathbb{Q}(\xi_n)$, and $\mathcal{O}_L$ be the ring of integers of L. Since $SOC(\mathcal{M}_n) \cong \{\gamma \in K : |\gamma| = 1\}$, a coincidence rotation R of $\mathcal{M}_n$ corresponds to multiplication by a complex number

$$\gamma = \varepsilon \cdot \prod_{k \in \mathcal{C}} \left(\frac{\omega_k}{\overline{\omega_k}}\right)^{n_k},$$

where ε is a root of unity in K (of the form $\pm\xi_n^j$ for $0 \leq j \leq n-1$), $n_k \in \mathbb{Z}$ and only a finite number of $n_k \neq 0$, $\mathcal{C}$ is the set of splitting primes of $\mathcal{O}_L$ over $\mathcal{M}_n$, and ω_k, $\overline{\omega_k}$ are the prime factors of $k \in \mathcal{C}$. Here, the CSM generated by R is the ideal $\mathcal{M}_n(R) = (z) = z\mathcal{M}_n$, where

$$z = \mathrm{num}(\gamma) = \begin{cases} 1, & \text{if } R \in P(\mathcal{M}_n) \\ \displaystyle\prod_{\substack{k \in \mathcal{C} \\ n_k > 0}} {w_k}^{n_k} \cdot \prod_{\substack{k \in \mathcal{C} \\ n_k < 0}} (\overline{w_k})^{-n_k}, & \text{otherwise,} \end{cases}$$

and the coincidence index of R with respect to $\mathcal{M}_n$ is equal to the absolute norm of z.

Thus, $SOC(\mathcal{M}_n) \cong C_N \times \mathbb{Z}^{(\aleph_0)}$, where C_N is the cyclic group of order N generated by ξ_n and $\mathbb{Z}^{(\aleph_0)}$ is the direct sum of countably many infinite cyclic groups each of which is generated by $\frac{\omega_k}{\overline{\omega_k}}$. In addition, $OC(\mathcal{M}_n) = SOC(\mathcal{M}_n) \rtimes \langle T_r \rangle$, where T_r again denotes complex conjugation.

The details of the discussion here can be found in [**59, 4, 11**].

Remark 1.12: An $R_{z,\varepsilon} \in SOC(\mathcal{M}_n)$ shall denote the coincidence rotation corresponding to multiplication by $\varepsilon\frac{z}{\bar{z}}$, while $T_{z,\varepsilon} \in OC(\mathcal{M}_n) \setminus SOC(\mathcal{M}_n)$ stands for the coincidence reflection $T_{z,\varepsilon} = R_{z,\varepsilon} \cdot T_r$.

1.2.3. Quaternions. Linear isometries in three and four dimensions can be parametrized by quaternions, which turns out to be a very useful tool in the solution of the coincidence problem for lattices and $\mathbb{Z}$-modules in both dimensions. We thus recall some essential properties of the quaternion algebra $\mathbb{H}(\mathbb{R})$ here. Extensive treatments on quaternions can be found in [**49, 18, 48, 43, 20**].

Let $\{\mathbf{e}, \mathbf{i}, \mathbf{j}, \mathbf{k}\}$ be the standard basis of $\mathbb{R}^4$ where $\mathbf{e} = (1,0,0,0)^T$, $\mathbf{i} = (0,1,0,0)^T$, $\mathbf{j} = (0,0,1,0)^T$, and $\mathbf{k} = (0,0,0,1)^T$. The *quaternion algebra* is the algebra $\mathbb{H} := \mathbb{H}(\mathbb{R}) = \mathbb{R}\mathbf{e} + \mathbb{R}\mathbf{i} + \mathbb{R}\mathbf{j} + \mathbb{R}\mathbf{k} \cong \mathbb{R}^4$ where multiplication is defined by the relations

$$\mathbf{i}^2 = \mathbf{j}^2 = \mathbf{k}^2 = \mathbf{ijk} = -1.$$

Elements of $\mathbb{H}$ are called *quaternions*, and a quaternion q is written as either $q = q_0\mathbf{e} + q_1\mathbf{i} + q_2\mathbf{j} + q_3\mathbf{k}$ or $q = (q_0, q_1, q_2, q_3)$. Given two quaternions $q = (q_0, q_1, q_2, q_3)$ and $p = (p_0, p_1, p_2, p_3)$, their product is given by the quaternion

$$q\,p = (q_0p_0 - q_1p_1 - q_2p_2 - q_3p_3)\mathbf{e} + (q_0p_1 + q_1p_0 + q_2p_3 - q_3p_2)\mathbf{i} + \\ (q_0p_2 - q_1p_3 + q_2p_0 + q_3p_1)\mathbf{j} + (q_0p_3 + q_1p_2 - q_2p_1 + q_3p_0)\mathbf{k}.$$

Multiplication of quaternions is associative but not commutative. The *inner product* of q and p is defined as the standard scalar product of q and p as vectors in $\mathbb{R}^4$, that is, $\langle q, p\rangle = \sum_{j=0}^{3} q_jp_j$.

The *conjugate* of a quaternion $q = (q_0, q_1, q_2, q_3)$ is $\overline{q} = (q_0, -q_1, -q_2, -q_3)$, and its *norm* is $|q|^2 = q\,\overline{q} = q_0^2 + q_1^2 + q_2^2 + q_3^2 \in \mathbb{R}$. It is easy to verify that $\overline{q\,p} = \overline{p}\,\overline{q}$ and $|q\,p|^2 = |q|^2|p|^2$ for any $q, p \in \mathbb{H}$. Every nonzero quaternion q has a multiplicative inverse given by $q^{-1} = \frac{\overline{q}}{|q|^2}$, which makes $\mathbb{H}$ an associative division algebra.

A quaternion whose components are all integers is called a *Lipschitz quaternion* or *Lipschitz integer*. The set of Lipschitz quaternions shall be denoted by

$$\mathbb{L} = \{(q_0, q_1, q_2, q_3) \in \mathbb{H} : q_0, q_1, q_2, q_3 \in \mathbb{Z}\}.$$

A *primitive quaternion* $q = (q_0, q_1, q_2, q_3)$ is a quaternion in $\mathbb{L}$ whose components are relatively prime, that is, $\gcd(q_0, q_1, q_2, q_3) = 1$. On the other hand, a *Hurwitz quaternion* or *Hurwitz integer* is a quaternion whose components are all integers or all half-integers. The set $\mathbb{J}$ of Hurwitz quaternions is given by

$$\begin{aligned}\mathbb{J} &= \left\{(q_0, q_1, q_2, q_3) \in \mathbb{H} : q_0, q_1, q_2, q_3 \in \mathbb{Z} \text{ or } q_0, q_1, q_2, q_3 \in \tfrac{1}{2} + \mathbb{Z}\right\} \\ &= \mathbb{L} \cup [(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}) + \mathbb{L}].\end{aligned}$$

The set $\mathbb{J}$ is in fact a maximal order in the division ring

$$\mathbb{H}(\mathbb{Q}) = \{(q_0, q_1, q_2, q_3) \in \mathbb{H} : q_0, q_1, q_2, q_3 \in \mathbb{Q}\}.$$

The following theorem, which appears in [**48**, page 37], describes the factorization of a Hurwitz quaternion whose norm is even, and will be of use in later calculations.

Theorem 1.13: *If $q \in \mathbb{J}$ and j is the highest power of 2 such that 2^j divides $|q|^2$, then $q = (1 + \mathbf{i})^j p$ for some $p \in \mathbb{J}$ of odd norm.*

For a quaternion $q = (q_0, q_1, q_2, q_3)$, its *real part* and *imaginary part* are defined as $\mathrm{Re}\,(q) = q_0$ and $\mathrm{Im}\,(q) = q_1\mathbf{i} + q_2\mathbf{j} + q_3\mathbf{k}$, respectively. The *imaginary space of* $\mathbb{H}$ is the three-dimensional vector subspace

$$\mathrm{Im}\,(\mathbb{H}) = \{\mathrm{Im}\,(q) : q \in \mathbb{H}\} = \mathbb{R}\mathbf{i} + \mathbb{R}\mathbf{j} + \mathbb{R}\mathbf{k} \cong \mathbb{R}^3,$$

of $\mathbb{H}$. Thus, $\mathbb{H}$ can be written as the direct product $\mathbb{H} = \mathbb{R}\mathbf{e} \oplus \mathrm{Im}\,(\mathbb{H})$. Given an $R \in SO(\mathrm{Im}\,(\mathbb{H})) \cong SO(3)$, there exists a quaternion q so that for all $x \in \mathrm{Im}\,(\mathbb{H})$, $R(x) = qxq^{-1}$. In such a case, we denote R by R_q. In the same manner, a quaternion q can be associated to every $T \in O(\mathrm{Im}\,(\mathbb{H})) \setminus SO(\mathrm{Im}\,(\mathbb{H}))$ so that $T(x) = q\overline{x}q^{-1} = -qxq^{-1}$ for all $x \in \mathrm{Im}\,(\mathbb{H})$, in which case, T shall be written as T_q.

As an element of $SO(3)$, a rotation R parametrized by the quaternion $q = (q_0, q_1, q_2, q_3)$ corresponds to the matrix

$$R_q = \frac{1}{|q|^2}\begin{pmatrix} q_0^2+q_1^2-q_2^2-q_3^2 & -2q_0q_3+2q_1q_2 & 2q_0q_2+2q_1q_3 \\ 2q_0q_3+2q_1q_2 & q_0^2-q_1^2+q_2^2-q_3^2 & -2q_0q_1+2q_2q_3 \\ -2q_0q_2+2q_1q_3 & 2q_0q_1+2q_2q_3 & q_0^2-q_1^2-q_2^2+q_3^2 \end{pmatrix}.$$

This defines a group homomorphism from $\mathbb{H}$ to $SO(3)$ given by $q \mapsto R_q$, called the *Cayley parametrization* of $SO(3)$. Similarly, a reflection T parametrized by the quaternion q corresponds to the matrix $T_q = -R_q$ in $O(3)$.

Elements of $O(4)$ can also be parametrized via quaternions. For every rotation $R \in SO(\mathbb{H}) \cong SO(4)$ and reflection $T \in O(\mathbb{H}) \setminus SO(\mathbb{H})$, there exists a pair of quaternions (q, p) so that $R(x) = \frac{1}{|q\,p|} qx\overline{p}$ and $T(x) = \frac{1}{|q\,p|} q\overline{x}\,\overline{p}$ for all $x \in \mathbb{H}$. From this point onwards, $R_{q,p} \in SO(\mathbb{H})$ and $T_{q,p} \in O(\mathbb{H}) \setminus SO(\mathbb{H})$ means that R and T are parametrized by the pair (q, p) of quaternions.

The rotation $R_{q,p} \in SO(\mathbb{H})$ with $q = (k, \ell, m, n)$ and $p = (a, b, c, d)$ corresponds to the matrix

$$R_{q,p} = \frac{1}{|q\,p|}\begin{pmatrix} ak+b\ell+cm+dn & -a\ell+bk+cn-dm & -am-bn+ck+d\ell & -an+bm-c\ell+dk \\ a\ell-bk+cn-dm & ak+b\ell-cm-dn & -an+bm+c\ell-dk & am+bn+ck+d\ell \\ am-bn-ck+d\ell & an+bm+c\ell+dk & ak-b\ell+cm-dn & -a\ell-bk+cn+dm \\ an+bm-c\ell-dk & -am+bn-ck+d\ell & a\ell+bk+cn+dm & ak-b\ell-cm+dn \end{pmatrix}$$

in $SO(4)$. Also, the rotoreflection $T \in O(\mathbb{H}) \setminus SO(\mathbb{H})$ parametrized by the quaternion pair (q, p) corresponds to the matrix $T_{q,p} = R_{q,p} \cdot T_{1,1}$, where

$$T_{1,1} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

1.2.4. Cubic lattices. Coincidences of cubic lattices are the most studied case because of their relevance to crystallography, see [**33, 34, 39, 36, 38, 4, 81**]. It suffices, however, to look at the primitive cubic lattice when studying the coincidences of the three-dimensional cubic lattices, namely, the primitive cubic, face-centered cubic, and body-centered cubic lattices, because of the following well-known result [**39, 4**].

Theorem 1.14: *Let $\Gamma_P = \mathbb{Z}^3$, $\Gamma_B = \Gamma_P \cup [(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) + \Gamma_P]$, and $\Gamma_F = \Gamma_B^*$ denote the primitive cubic, body-centered cubic, and face-centered cubic lattice, respectively. Then $OC(\Gamma_P) = OC(\Gamma_F) = OC(\Gamma_B) = O(3, \mathbb{Q})$. Moreover, if $R \in O(3, \mathbb{Q})$, then $\Sigma_{\Gamma_P}(R) = \Sigma_{\Gamma_F}(R) = \Sigma_{\Gamma_B}(R)$.*

Note that it is enough to take the primitive cubic lattice Γ to be $\mathbb{Z}^3$ because any other primitive cubic lattice is similar to $\mathbb{Z}^3$. As in the planar case, the analysis of $OC(\Gamma) = O(3, \mathbb{Q})$ starts with the set of coincidence rotations of Γ, $SO(3, \mathbb{Q})$, since $O(3)$ is the direct product of $SO(3)$ and $\{\pm\mathbb{1}_3\}$, where $\mathbb{1}_3$ is the 3×3-identity matrix. To this end, Cayley's parametrization of rotations in $SO(3)$ by quaternions is used [**4**].

Since $R_{tq} = R_q$ for every $t \in \mathbb{R} \setminus \{0\}$, every $R \in SOC(\Gamma) = SO(3, \mathbb{Q})$ can be parametrized by a primitive quaternion. Even though this method exhausts $SO(3, \mathbb{Q})$, each element of $SO(3,\mathbb{Q})$ is encountered twice because $R_{-q} = R_q$. The coincidence index of $R_q \in SOC(\Gamma)$, with q primitive, is equal to the odd part of $|q|^2$, that is, $\Sigma(R_q) = \frac{|q|^2}{2^\ell}$, where ℓ is the largest power of 2 that divides $|q|^2$ [**39, 38, 4**].

Write $T_q \in O(3) \setminus SO(3)$ as $T = R_q \cdot (-\mathbb{1}_3)$, where $R_q \in SO(3)$. Then the quaternion q can also be chosen such that it is primitive whenever $T_q \in OC(\Gamma)$, because the inversion $-\mathbb{1}_3$ fixes Γ. In addition, $\Sigma(T_q) = \Sigma(R_q)$ and $\Gamma(T_q) = \Gamma(R_q)$.

Let $f_{\mathbb{Z}^3}(m)$ be the number of CSLs of $\mathbb{Z}^3$ of index m. Once again, $f_{\mathbb{Z}^3}$ is multiplicative and is given by

$$f_{\mathbb{Z}^3}(p^r) = \begin{cases} 0, & \text{if } p = 2 \\ (p+1)p^{r-1}, & \text{otherwise,} \end{cases}$$

where p is prime and $r \in \mathbb{N}$ [**38, 4**]. From this, one obtains the Dirichlet series generating function for $f_{\mathbb{Z}^3}$, namely,

$$\begin{aligned} \Phi_{\mathbb{Z}^3}(s) &= \sum_{m=1}^{\infty} \frac{f_{\mathbb{Z}^3}(m)}{m^s} = \prod_{p \neq 2} \left(1 + \frac{p+1}{p^s} + \frac{(p+1)p}{p^{2s}} + \ldots\right) = \prod_{p \neq 2} \frac{1+p^{-s}}{1-p^{1-s}} \\ &= 1 + \tfrac{4}{3^s} + \tfrac{6}{5^s} + \tfrac{8}{7^s} + \tfrac{12}{9^s} + \tfrac{12}{11^s} + \tfrac{14}{13^s} + \tfrac{24}{15^s} + \tfrac{18}{17^s} + \tfrac{20}{19^s} \\ &\quad + \tfrac{32}{21^s} + \tfrac{24}{23^s} + \cdots . \end{aligned} \tag{1.4}$$

One sees from (1.4) that the set of coincidence indices of the cubic lattices is the set of odd natural numbers. Since $\mathbb{Z}^3$ has twenty-four symmetry rotations, the number of coincidence rotations of index m is given by $\hat{f}_{\mathbb{Z}^3}(m) = 24 f_{\mathbb{Z}^3}(m)$, and the Dirichlet series generating function for $\hat{f}_{\mathbb{Z}^3}(m)$ is $24\Phi_{\mathbb{Z}^3}(s)$.

1.2.5. Hypercubic lattices. The discovery of quasicrystals sparked interest on the coincidence problem for higher-dimensional lattices. The coincidences of the hypercubic lattices are described in this part, based on the discussion in [**4, 82, 13**]. In the following, elements of $O(4)$ are parametrized by pairs of quaternions.

There are only two distinct types of hypercubic lattices in four dimensions, namely the primitive hypercubic lattice $\mathbb{Z}^4$ and the centered hypercubic lattice D_4. Even though $OC(\mathbb{Z}^4) = OC(D_4) = O(4,\mathbb{Q})$, the coincidence indices of a coincidence isometry with respect to the two lattices are not necessarily equal. This is evident from the fact that the point symmetry group of D_4 is three times larger than that of $\mathbb{Z}^4$. Thus, we deal with the coincidences of the two lattices separately.

A rotation $R_{q,p} \in SOC(D_4) = SO(4,\mathbb{Q})$ if and only if q and p are primitive quaternions satisfying $|q\,p| \in \mathbb{Z}$. Such pairs of quaternions shall be called *admissible*. Note that $R_{-q,-p} = R_{q,p}$, and thus each element of $SO(4,\mathbb{Q})$ is obtained twice when all admissible pairs of quaternions are considered. The coincidence index of $R_{q,p} \in SOC(D_4)$ is given by $\Sigma_{D_4}(R_{q,p}) = \mathrm{lcm}\left(\frac{|q|^2}{2^k}, \frac{|p|^2}{2^\ell}\right)$, where k and ℓ are the highest powers such that 2^k and 2^ℓ divide $|q|^2$ and $|p|^2$, respectively. It follows that the set of coincidence indices of D_4 is the set of all odd numbers.

Since the reflection $T_{1,1}$ leaves D_4 invariant, every reflection in $OC(4,\mathbb{Q})$ can also be parametrized by an admissible pair of quaternions. Furthermore, if $T_{q,p} = R_{q,p} \cdot T_{1,1} \in OC(4,\mathbb{Q}) \setminus SOC(4,\mathbb{Q})$ then $\Sigma_{D_4}(T_{q,p}) = \Sigma_{D_4}(R_{q,p})$ and $D_4(T_{q,p}) = D_4(R_{q,p})$.

The *denominator* of a matrix $R \in O(d)$ is defined as

$$\mathrm{den}(R) = \gcd\{k \in \mathbb{N} : k\,R \text{ is an integral matrix}\}. \tag{1.5}$$

With this on hand, one can now compute for the coincidence index of $R_{q,p} \in SO(4,\mathbb{Q})$ with respect to $\mathbb{Z}^4$. Since $\mathbb{Z}^4$ is a sublattice of D_4 of index 2, either $\Sigma_{\mathbb{Z}^4}(R_{q,p}) = \Sigma_{D_4}(R_{q,p})$ or $\Sigma_{\mathbb{Z}^4}(R_{q,p}) = 2\,\Sigma_{D_4}(R_{q,p})$. Both situations in fact occur, and explicitly one has

$$\Sigma_{\mathbb{Z}^4}(R_{q,p}) = \mathrm{lcm}(\Sigma_{D_4}(R_{q,p}), \mathrm{den}(R_{q,p})). \tag{1.6}$$

The same result holds true for coincidence reflections $T_{q,p}$ of $\mathbb{Z}^4$.

1.3. Lattice colorings

Various equivalent definitions and notions involving colorings of lattices abound in the literature, see [**74, 70, 41, 71, 69, 58**]. Here we focus on the definitions and relevant results that will be used in this thesis.

Let Γ_1 be a lattice in $\mathbb{R}^d$. A *coloring* of Γ_1 by m colors is an onto mapping $c : \Gamma_1 \to C$, where C is the set of m colors used in the coloring. Of particular interest in this thesis are colorings of Γ_1 by m colors wherein two points of Γ_1 are assigned the same color if and only if they belong to the same coset of some sublattice Γ_2 of index m in Γ_1. Such a coloring shall be referred to as a *coloring of* Γ_1 *determined by the sublattice* Γ_2. Here, the set of colors C can be identified with the quotient group Γ_1/Γ_2 so that the color mapping c is just the canonical projection of Γ_1 onto Γ_1/Γ_2 whose kernel is Γ_2. Subsequently, we simply take $C = \{c_0 = 0, c_1, \ldots, c_{m-1}\}$ to be a complete set of coset representatives of Γ_2 in Γ_1, and say that the coset $c_j + \Gamma_2$ has color c_j.

Denote by G the symmetry group of Γ_1 and fix a coloring c of Γ_1. A symmetry in G is called a *color symmetry* of the coloring if it permutes the colors in the coloring, that is, all and only those points having the same color are mapped by the symmetry to a fixed color. The set H of all color symmetries of the coloring, that is,

$$H = \{h \in G : \exists\, \sigma_h \in S_C \text{ such that } \forall\, \ell \in \Gamma_1, c(h(\ell)) = \sigma_h(c(\ell))\},$$

where S_C is the set of permutations on the set of colors C, forms a group and is called the *color group* or *color symmetry group* of the coloring. The mapping $P : H \to S_C$ with $h \mapsto \sigma_h$ defines a group homomorphism, and thus the group H acts on C. The kernel of P,

$$K = \{k \in H : c(k(\ell)) = c(\ell),\, \forall\, \ell \in \Gamma_1\},$$

is the subgroup of H whose elements fix the colors in the coloring. In other words, K is the symmetry group of the colored lattice. For this reason, the group K is referred to as the *color preserving group* or the *color fixing group* of the coloring. By the first isomorphism theorem, the group of color permutations of the coloring, $P(H)$, is isomorphic to H/K. The short exact sequence

$$0 \longrightarrow K \longrightarrow H \longrightarrow H/K \longrightarrow 0$$

summarizes the relationship of the groups H, K, and H/K.

CHAPTER 2

Coincidence indices of sublattices and colorings of lattices

In this chapter, we examine the relationship between the coincidence indices of a lattice Γ_1 and the coincidence indices of a sublattice Γ_2 of Γ_1 via the coloring of Γ_1 determined by Γ_2. In addition, the idea of color symmetry, originally defined for symmetries of lattices, is extended to coincidence isometries of lattices. Some of the results in this chapter, including examples involving lattices and $\mathbb{Z}$-modules in the plane, can be found in [**52**].

Unless otherwise stated, Γ_1 is taken throughout this chapter to be a lattice having Γ_2 as a sublattice of index m. We write $\Gamma_1 = \bigcup_{j=0}^{m-1} (c_j + \Gamma_2)$ with $c_0 = 0$, and consider the coloring of Γ_1 determined by Γ_2.

2.1. Coincidence index with respect to a sublattice

Fix an $R \in OC(\Gamma_1) = OC(\Gamma_2)$. Consider the following subgroups of Γ_1/Γ_2:

$$\begin{aligned} J &:= \left\{ c_j + \Gamma_2 : (c_j + \Gamma_2) \cap \Gamma_1(R^{-1}) \neq \varnothing \right\}, \\ K &:= \left\{ c_k + \Gamma_2 : (c_k + \Gamma_2) \cap \Gamma_1(R) \neq \varnothing \right\} \end{aligned} \tag{2.1}$$

The sets J and K are nonempty because both sets have $c_0 + \Gamma_2 = \Gamma_2$ as an element. These sets induce partitions of $\Gamma_1(R^{-1})$ and $\Gamma_1(R)$, respectively, given by

$$\begin{aligned} \Gamma_1(R^{-1}) &= \bigcup_{c_j + \Gamma_2 \in J} (c_j + \Gamma_2) \cap \Gamma_1(R^{-1}) \text{ and} \\ \Gamma_1(R) &= \bigcup_{c_k + \Gamma_2 \in K} (c_k + \Gamma_2) \cap \Gamma_1(R). \end{aligned} \tag{2.2}$$

The partitions in (2.2) correspond to colorings of $\Gamma_1(R^{-1})$ and $\Gamma_1(R)$, respectively, wherein the colors are inherited from the coloring of Γ_1 determined by Γ_2. We shall refer to these colorings as the *colorings of* $\Gamma_1(R^{-1})$ *and* $\Gamma_1(R)$ *determined by* Γ_2. The set of colors in the colorings of $\Gamma_1(R^{-1})$ and $\Gamma_1(R)$ are

$$C_{R^{-1}} := \{c_j : c_j + \Gamma_2 \in J\} \qquad \text{and} \qquad C_R := \{c_k : c_k + \Gamma_2 \in K\}, \tag{2.3}$$

respectively. The coincidence isometry R determines a relation σ from $C_{R^{-1}}$ to C_R given by

$$\sigma = \left\{ (c_j, c_k) \in C_{R^{-1}} \times C_R : R[(c_j + \Gamma_2) \cap \Gamma_1(R^{-1})] \cap [(c_k + \Gamma_2) \cap \Gamma_1(R)] \neq \varnothing \right\}. \tag{2.4}$$

That is, $(c_j, c_k) \in \sigma$ means that some of the points colored c_j in the coloring of $\Gamma_1(R^{-1})$ are brought by R to points with color c_k in the coloring of $\Gamma_1(R)$. Since all points of $\Gamma_1(R^{-1})$ are mapped bijectively by R to points of $\Gamma_1(R)$ by Proposition 1.2, the relation σ is never empty. In fact, $(c_0, c_0) \in \sigma$ because the lattices $R[\Gamma_2 \cap \Gamma_1(R^{-1})] = R\Gamma_2 \cap \Gamma_1(R)$ and $\Gamma_2 \cap \Gamma_1(R)$ are commensurate.

REMARK 2.1:

(i) From each $c_j + \Gamma_2 \in J$, we can always choose a suitable coset representative $\tilde{c}_j$ such that $\tilde{c}_j + \Gamma_2 = c_j + \Gamma_2$ with $\tilde{c}_j \in \Gamma_1(R^{-1})$. Similarly, for every $c_k + \Gamma_2 \in K$, there exists $\tilde{\tilde{c}}_k$ satisfying $\tilde{\tilde{c}}_k + \Gamma_2 = c_k + \Gamma_2$ with $\tilde{\tilde{c}}_k \in \Gamma_1(R)$.

(ii) Given a coset $c_\ell + \Gamma_2 \neq \Gamma_2$ that is both in J and K, it may happen that $(c_\ell + \Gamma_2) \cap \Gamma_1(R^{-1}) \cap \Gamma_1(R) = \varnothing$. In such a case, it is not possible to find a coset representative $c_\ell{}'$ of $c_\ell + \Gamma_2$ having the property $c_\ell{}' + \Gamma_2 = c_\ell + \Gamma_2$ with $c_\ell{}' \in \Gamma_1(R^{-1}) \cap \Gamma_1(R)$.

The following lemma tells us that $\Gamma_2(R)$ consists of those points colored c_0 in the coloring of $\Gamma_1(R)$ whose preimages under R are also points colored c_0 in the coloring of $\Gamma_1(R^{-1})$.

Lemma 2.2: *Let Γ_2 be a sublattice of Γ_1 and $R \in OC(\Gamma_1)$. Then the lattices $\Gamma_2 \cap \Gamma_1(R)$ and $R\Gamma_2 \cap \Gamma_1(R)$ are commensurate with intersection $\Gamma_2(R)$. In particular, if $R\Gamma_2 \cap \Gamma_1(R) = \Gamma_2 \cap \Gamma_1(R)$ then $\Gamma_2(R) = R\Gamma_2 \cap \Gamma_1(R) = \Gamma_2 \cap \Gamma_1(R)$.*

Proof: One has $[\Gamma_2 \cap \Gamma_1(R)] \cap [R\Gamma_2 \cap \Gamma_1(R)] = (\Gamma_2 \cap R\Gamma_2) \cap \Gamma_1(R) = \Gamma_2(R)$. ■

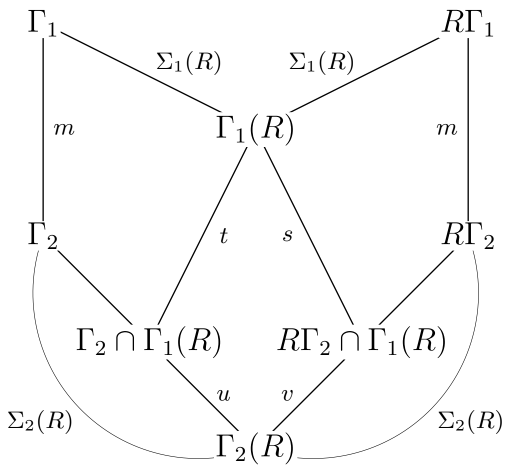


FIGURE 2. Lattice diagram of the lattices Γ_1, $R\Gamma_1$, Γ_2, $R\Gamma_2$, $\Gamma_1(R)$, $\Gamma_2(R)$, $\Gamma_2 \cap \Gamma_1(R)$, and $R\Gamma_2 \cap \Gamma_1(R)$ (as groups) and corresponding indices

Figure 2 exhibits the relationships among the various lattices. The following notations shall be used to indicate the corresponding lattice indices (see Figure 2):

$$\begin{aligned} s &:= [\Gamma_1(R) : R\Gamma_2 \cap \Gamma_1(R)] \quad , \quad & u &:= [\Gamma_2 \cap \Gamma_1(R) : \Gamma_2(R)] \\ t &:= [\Gamma_1(R) : \Gamma_2 \cap \Gamma_1(R)] \quad , \quad & v &:= [R\Gamma_2 \cap \Gamma_1(R) : \Gamma_2(R)] \end{aligned} \tag{2.5}$$

The next lemma is a consequence of the second isomorphism theorem and will be used repeatedly in the proof of the succeeding theorem.

Lemma 2.3: *Let Γ_2 and Γ_2' be sublattices of the lattice Γ_1. Then the following holds.*

(i) $[\Gamma_2' : \Gamma_2 \cap \Gamma_2'] = |\{\ell + \Gamma_2 \in \Gamma_1/\Gamma_2 : (\ell + \Gamma_2) \cap \Gamma_2' \neq \varnothing\}|$,

(ii) $[\Gamma_2' : \Gamma_2 \cap \Gamma_2']$ *divides* $[\Gamma_1 : \Gamma_2]$,

(iii) *If* $(\ell + \Gamma_2) \cap \Gamma_2' \neq \varnothing$ *then* $(\ell + \Gamma_2) \cap \Gamma_2'$ *is the coset* $\dot{\ell} + (\Gamma_2 \cap \Gamma_2')$ *of* $\Gamma_2 \cap \Gamma_2'$ *in* Γ_2' *whenever* $\dot{\ell} \in (\ell + \Gamma_2) \cap \Gamma_2'$.

Proof: From the second isomorphism theorem,

$$\Gamma_2'/(\Gamma_2 \cap \Gamma_2') \cong (\Gamma_2 + \Gamma_2')/\Gamma_2 = \{\ell + \Gamma_2 \in \Gamma_1/\Gamma_2 : (\ell + \Gamma_2) \cap \Gamma_2' \neq \varnothing\},$$

and this proves (i).

Since $\Gamma_2 + \Gamma_2'$ is a sublattice of Γ_1, $(\Gamma_2 + \Gamma_2')/\Gamma_2$ is a subgroup of Γ_1/Γ_2. Thus, $[\Gamma_2 + \Gamma_2' : \Gamma_2] = [\Gamma_2' : \Gamma_2 \cap \Gamma_2']$ divides $[\Gamma_1 : \Gamma_2]$ by Lagrange's Theorem.

The last statement is clear by replacing $\ell + \Gamma_2$ by $\dot{\ell} + \Gamma_2$. ∎

Using Lemma 2.3, one can now give restrictions on the values of s, t, u, and v, as well as interpretations of these values in relation to the colorings of $\Gamma_1(R^{-1})$ and $\Gamma_1(R)$ determined by Γ_2. These results are explicitly stated in the following theorem.

Theorem 2.4: *Consider the coloring of a lattice Γ_1 determined by a sublattice Γ_2 of Γ_1 of index m where each coset $c_j + \Gamma_2$ is assigned the color c_j for $0 \leq j \leq m-1$, with $c_0 = 0$. If $R \in OC(\Gamma_1)$, then*

$$\Sigma_2(R) = \frac{t \cdot u \cdot \Sigma_1(R)}{m} = \frac{s \cdot v \cdot \Sigma_1(R)}{m}, \tag{2.6}$$

where s and t are the number of colors in the coloring of $\Gamma_1(R^{-1})$ and $\Gamma_1(R)$, respectively, determined by Γ_2; u is the number of colors c_j with the property that some points of $\Gamma_1(R^{-1})$ colored c_j are mapped by R to points colored c_0 in the coloring of $\Gamma_1(R)$; and v is the number of colors in the coloring of $\Gamma_1(R)$ that is intersected by the images under R of those points of $\Gamma_1(R^{-1})$ colored c_0. Moreover, $s \mid m$, $t \mid m$, $u \mid s$, and $v \mid t$.

Proof: Comparing indices in Figure 2 gives the formula for $\Sigma_2(R)$ in terms of $\Sigma_1(R)$ in (2.6).

Take the sublattices Γ_2 and $\Gamma_1(R)$ of Γ_1. Applying Lemma 2.3, one readily obtains that $t = |K| = |C_R|$ (see (2.1) and (2.3)) and $t \mid m$. Corresponding statements for s are similarly proved by looking at the sublattices $R\Gamma_2$ and $\Gamma_1(R)$ of $R\Gamma_1$. Lemma 2.3 also implies that for all $c_j + \Gamma_2 \in J$ and $c_k + \Gamma_2 \in K$,

$$\begin{gathered} R[(c_j + \Gamma_2) \cap \Gamma_1(R^{-1})] = R\tilde{c}_j + [R\Gamma_2 \cap \Gamma_1(R)] \text{ and} \\ (c_k + \Gamma_2) \cap \Gamma_1(R) = \tilde{\tilde{c}}_k + [\Gamma_2 \cap \Gamma_1(R)], \end{gathered} \tag{2.7}$$

for some $\tilde{c}_j \in (c_j + \Gamma_2) \cap \Gamma_1(R^{-1})$ and $\tilde{\tilde{c}}_k \in (c_k + \Gamma_2) \cap \Gamma_1(R)$ (see Remark 2.1).

To complete the proof, consider the following sets:

$$\begin{aligned} D &:= \{R\tilde{c}_j + [R\Gamma_2 \cap \Gamma_1(R)] : c_j + \Gamma_2 \in J \text{ with } (R\tilde{c}_j + [R\Gamma_2 \cap \Gamma_1(R)]) \cap [\Gamma_2 \cap \Gamma_1(R)] \neq \varnothing\} \\ E &:= \left\{\tilde{\tilde{c}}_k + [\Gamma_2 \cap \Gamma_1(R)] : c_k + \Gamma_2 \in K \text{ with } \left(\tilde{\tilde{c}}_k + [\Gamma_2 \cap \Gamma_1(R)]\right) \cap [R\Gamma_2 \cap \Gamma_1(R)] \neq \varnothing\right\}. \end{aligned} \tag{2.8}$$

The sets D and E are never empty because the lattices $R\Gamma_2 \cap \Gamma_1(R)$ and $\Gamma_2 \cap \Gamma_1(R)$ are commensurate. From (2.4) and (2.7), one obtains $|D| = |\{c_j : (c_j, c_0) \in \sigma\}|$ and $|E| = |\{c_k : (c_0, c_k) \in \sigma\}|$.

Finally, consider the sublattices $\Gamma_2 \cap \Gamma_1(R)$ and $R\Gamma_2 \cap \Gamma_1(R)$ of $\Gamma_1(R)$. Invoking Lemma 2.3 twice gives $u = |D|$ with $u \mid s$, and $v = |E|$ with $v \mid t$. ■

REMARK 2.5: Lemma 2.3, when applied to the sublattices $\Gamma_2 \cap \Gamma_1(R)$ and $R\Gamma_2 \cap \Gamma_1(R)$ of $\Gamma_1(R)$, also implies that

$$(R\tilde{c}_j + [R\Gamma_2 \cap \Gamma_1(R)]) \cap [\Gamma_2 \cap \Gamma_1(R)] = R\tilde{c}_j + \Gamma_2(R), \text{ and}$$
$$\left(\tilde{\tilde{c}}_k + [\Gamma_2 \cap \Gamma_1(R)]\right) \cap [R\Gamma_2 \cap \Gamma_1(R)] = \tilde{\tilde{c}}_k + \Gamma_2(R),$$

for all $R\tilde{c}_j + [R\Gamma_2 \cap \Gamma_1(R)] \in D$ whenever $R\tilde{c}_j \in \Gamma_2 \cap \Gamma_1(R)$, and $\tilde{\tilde{c}}_k + [\Gamma_2 \cap \Gamma_1(R)] \in E$ whenever $\tilde{\tilde{c}}_k \in R\Gamma_2 \cap \Gamma_1(R)$.

An immediate consequence of Theorem 2.4 are the following divisibility conditions on the value of $\Sigma_2(R)$: $\Sigma_1(R) \mid m\,\Sigma_2(R)$ and $\Sigma_2(R) \mid m\,\Sigma_1(R)$ (see Proposition 1.7 and Remark 1.8). Both conditions imply the well-known bound on $\Sigma_2(R)$: $\frac{1}{m}\Sigma_1(R) \leq \Sigma_2(R) \leq m\,\Sigma_1(R)$. Also, observe that $s = t$ if and only if $u = v$.

One should note that the divisibility condition $\Sigma_2(R) \mid m\,\Sigma_1(R)$, and hence, the inequality $\Sigma_2(R) \leq m\,\Sigma_1(R)$, was obtained here without going through the dual lattices of Γ_1 and Γ_2 (see Remark 1.8). This means that the said divisiblity condition is true not only for lattices but also for $\mathbb{Z}$-modules by Remark 1.10. This fact was not known to hold for all $\mathbb{Z}$-modules, because the dual of a $\mathbb{Z}$-module is not always defined (see end of Section 1.1).

EXAMPLE 2.6: Consider the square lattice $\Gamma_1 = \mathbb{Z}[i]$, and the sublattice Γ_2 of index 6 in Γ_1 generated by 6 and $2+i$, denoted as $\Gamma_2 = \langle 6, 2+i \rangle_{\mathbb{Z}}$. Take $R = R_{1+2i,-i} \in SOC(\Gamma_1)$ (see Remark 1.11), which corresponds to the rotation about the origin by $\tan^{-1}(\frac{3}{4}) \approx 37°$ in the counterclockwise direction. It is known that $\Sigma_1(R) = N(1+2i) = 5$. Choose the coset representatives $c_j = j$ for $0 \leq j \leq 5$ so that $\Gamma_1 = \bigcup_{j=0}^{5}(c_j + \Gamma_2)$. Colorings of Γ_1, $\Gamma_1(R^{-1})$, and $\Gamma_1(R)$ determined by Γ_2 are shown in Figures 3, 4(a), and 4(b). They were obtained by designating the colors black, yellow, blue, red, gray, and green to the cosets $c_0 + \Gamma_2$, $c_1 + \Gamma_2$, $c_2 + \Gamma_2$, $c_3 + \Gamma_2$, $c_4 + \Gamma_2$, and $c_5 + \Gamma_2$, respectively.

Since all six colors appear in both colorings of $\Gamma_1(R^{-1})$ and $\Gamma_1(R)$, $s = t = 6$ in (2.5). Observe that half of the black dots in the coloring of $\Gamma_1(R^{-1})$ are sent by R again to black dots in the coloring of $\Gamma_1(R)$, while the other half of the black dots are sent to red dots. This implies that $u = 2$. Therefore, by (2.6), $\Sigma_2(R) = \frac{6\cdot 2\cdot 5}{6} = 10$. By Lemma 2.2, $\Gamma_2(R)$ is the intersection of $\Gamma_2 \cap \Gamma_1(R)$ (the black dots in the coloring of $\Gamma_1(R)$) and $R[\Gamma_2 \cap \Gamma_1(R^{-1})]$ (the resulting dots when the black dots in the coloring of $\Gamma_1(R^{-1})$ are rotated by R). Points on the CSL $\Gamma_2(R)$ is shown in Figure 4(c) (black dots).

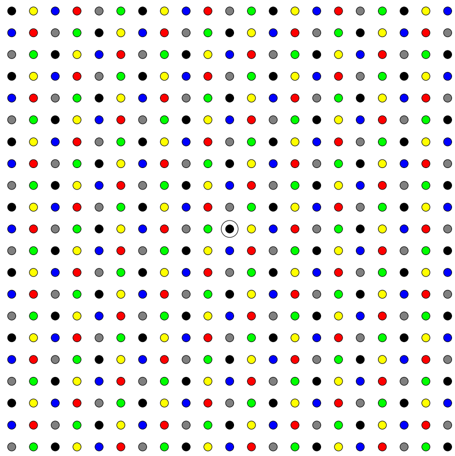


FIGURE 3. Coloring of the square lattice $\Gamma_1 = \mathbb{Z}[i]$ determined by the sublattice $\Gamma_2 = \langle 6, 2+i\rangle_{\mathbb{Z}}$(= black dots). The encircled dot indicates the origin.

2.2. Color coincidence

We have seen from the previous section how the interaction of the colors in the colorings of $\Gamma_1(R^{-1})$ and $\Gamma_1(R)$ determined by Γ_2 affects the formation of the lattice $\Gamma_2(R)$ and thus, the value of $\Sigma_2(R)$. This motivates the following definition.

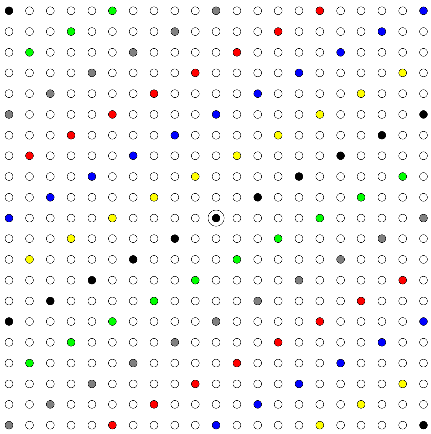
Definition 2.7: Let Γ_2 be a sublattice of Γ_1 and write $\Gamma_1 = \bigcup_{j=0}^{m-1}(c_j + \Gamma_2)$, with $c_0 = 0$. A coincidence isometry R of Γ_1 is said to be a *color coincidence* of the coloring of Γ_1 determined by Γ_2 if R defines a bijection between the partitions $\{(c_j + \Gamma_2) \cap \Gamma_1(R^{-1}) : c_j + \Gamma_2 \in J\}$ of $\Gamma_1(R^{-1})$ and $\{(c_k + \Gamma_2) \cap \Gamma_1(R) : c_k + \Gamma_2 \in K\}$ of $\Gamma_1(R)$ given by

$$R[(c_j + \Gamma_2) \cap \Gamma_1(R^{-1})] = (c_k + \Gamma_2) \cap \Gamma_1(R). \tag{2.9}$$

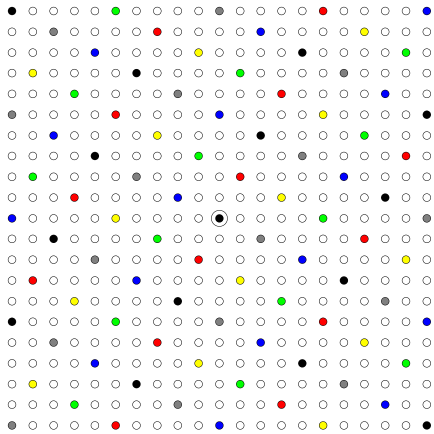
Condition (2.9) means that all points, and only those points, colored c_j in the coloring of $\Gamma_1(R^{-1})$ are mapped by R to points colored c_k in the coloring of $\Gamma_1(R)$. Whenever (2.9) is satisfied, R is said to send or map color c_j to color c_k. Furthermore, if R maps a color c_j onto itself, R is said to *fix the color* c_j. An $R \in OC(\Gamma_1)$ is then a color coincidence of the coloring of Γ_1 if the associated relation σ from $C_{R^{-1}}$ to C_R in (2.4) is a bijection. In particular, σ is a permutation on $C_{R^{-1}}$ for color coincidences R with $C_{R^{-1}} = C_R$. Thus, a color coincidence $R \in P(\Gamma_1)$ (that is, when $\Gamma_1(R^{-1}) = \Gamma_1(R) = \Gamma_1$) is a color symmetry of the coloring of Γ_1.

The next theorem, which is a generalization of the first result in [**19**, Theorem 2] on color symmetries of colorings of square and hexagonal lattices, provides a characterization of color coincidences of lattice colorings determined by some sublattice.

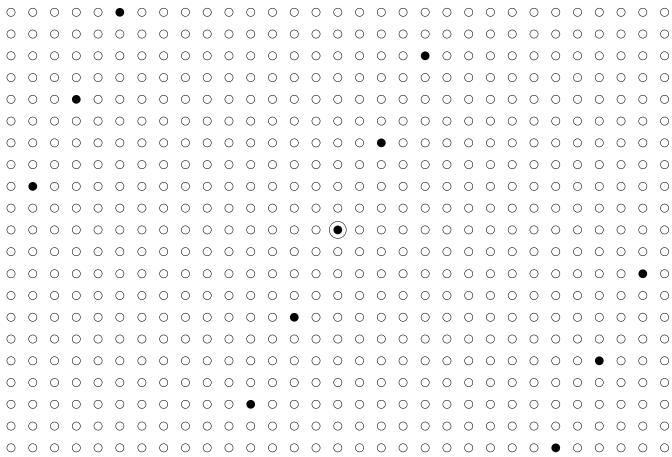
Theorem 2.8: *Let Γ_2 be a sublattice of Γ_1 with $\Gamma_1 = \bigcup_{j=0}^{m-1}(c_j + \Gamma_2)$ where $c_0 = 0$. Then $R \in OC(\Gamma_1)$ is a color coincidence of the coloring of Γ_1 determined by Γ_2 if and only if R fixes color c_0.*



(a) Coloring of $\Gamma_1(R^{-1})$ (white dots correspond to points of $\Gamma_1 \setminus \Gamma_1(R^{-1})$)



(b) Coloring of $\Gamma_1(R)$



(c) $\Gamma_2(R)$ (= black dots) as a sublattice of Γ_1.

FIGURE 4. Colorings of $\Gamma_1(R^{-1})$ and $\Gamma_1(R)$ determined by the sublattice Γ_2 of Figure 3, where R is the counterclockwise rotation about the origin by $\tan^{-1}(\frac{3}{4}) \approx 37°$. The CSL $\Gamma_2(R)$ of index 10 in Γ_2 is obtained by taking all black points of $\Gamma_1(R)$ whose preimages under R are also colored black.

Proof: Let R be a color coincidence of the coloring of Γ_1. The color c_0 appears in the coloring of $\Gamma_1(R^{-1})$ and R sends color c_0 to exactly one color c_k in the coloring of $\Gamma_1(R)$. Hence, $R[\Gamma_2 \cap \Gamma_1(R^{-1})] = (c_k + \Gamma_2) \cap \Gamma_1(R)$. Since $0 \in \Gamma_2 \cap \Gamma_1(R^{-1})$ and $R(0) = 0$, $0 \in (c_k + \Gamma_2) \cap \Gamma_1(R)$ which implies that $c_k = c_0$. Thus, R fixes color c_0.

In the other direction, suppose R fixes color c_0, that is, $R[\Gamma_2 \cap \Gamma_1(R^{-1})] = \Gamma_2 \cap \Gamma_1(R)$. This means that $\Gamma_2(R) = R\Gamma_2 \cap \Gamma_1(R) = \Gamma_2 \cap \Gamma_1(R)$ by Lemma 2.2. Hence, $u = v = 1$ and $s = t$ (refer to (2.5)). From Theorem 2.4, the colorings of $\Gamma_1(R)$ and $\Gamma_1(R^{-1})$ must have the same number of colors. Now, for each $c_j + \Gamma_2 \in J$, choose $\tilde{c}_j \in (c_j + \Gamma_2) \cap \Gamma_1(R^{-1})$. Then $R\tilde{c}_j + \Gamma_2 \in K$ with $R\tilde{c}_j \in \Gamma_1(R)$, and

$$R[(c_j + \Gamma_2) \cap \Gamma_1(R^{-1})] \underset{(2.7)}{=} R\tilde{c}_j + [R\Gamma_2 \cap \Gamma_1(R)] = R\tilde{c}_j + [\Gamma_2 \cap \Gamma_1(R)] \underset{(2.7)}{=} (R\tilde{c}_j + \Gamma_2) \cap \Gamma_1(R).$$

This means that $R\tilde{c}_j + \Gamma_2$ must be one of the cosets $c_k + \Gamma_2 \in K$. Therefore, R is a color coincidence of the coloring of Γ_1. ■

It follows from Theorem 2.8 that it is sufficient to verify whether $R[\Gamma_2 \cap \Gamma_1(R^{-1})] = \Gamma_2 \cap \Gamma_1(R)$ is satisfied or not to conclude whether $R \in OC(\Gamma_1)$ is a color coincidence of the coloring of the lattice Γ_1 induced by the sublattice Γ_2 of Γ_1.

REMARK 2.9: Let R be a color coincidence of the coloring of Γ_1 determined by Γ_2. It follows from (2.7), Lemma 2.2, and Theorem 2.8 that for all $c_j + \Gamma_2 \in J$ and $c_k + \Gamma_2 \in K$,

$$R[(c_j + \Gamma_2) \cap \Gamma_1(R^{-1})] = R\tilde{c}_j + [R\Gamma_2 \cap \Gamma_1(R)] = R\tilde{c}_j + \Gamma_2(R), \text{ and}$$
$$(c_k + \Gamma_2) \cap \Gamma_1(R) = \tilde{\tilde{c}}_k + [\Gamma_2 \cap \Gamma_1(R)] = \tilde{\tilde{c}}_k + \Gamma_2(R),$$

for some $\tilde{c}_j \in (c_j + \Gamma_2) \cap \Gamma_1(R^{-1})$ and $\tilde{\tilde{c}}_k \in (c_k + \Gamma_2) \cap \Gamma_1(R)$. This, together with (2.2), yields the following coset decompositions of $\Gamma_1(R)$ with respect to $\Gamma_2(R)$:

$$\Gamma_1(R) = \bigcup_{c_j+\Gamma_2 \in J} [R\tilde{c}_j + \Gamma_2(R)] = \bigcup_{c_k+\Gamma_2 \in K} \left[\tilde{\tilde{c}}_k + \Gamma_2(R)\right]$$

Hence, a color coincidence R determines a permutation on the set of cosets of $\Gamma_2(R)$ in $\Gamma_1(R)$. Here, $R\tilde{c}_j + \Gamma_2(R) = \tilde{\tilde{c}}_k + \Gamma_2(R)$ if and only if R sends color c_j to c_k.

The following corollaries link the property that a coincidence isometry R of Γ_1 is a color coincidence of the coloring of Γ_1 determined by Γ_2 with the relationship between $\Sigma_1(R)$ and $\Sigma_2(R)$.

Corollary 2.10: *If R is a color coincidence of the coloring of the lattice Γ_1 determined by the sublattice Γ_2, then $\Sigma_2(R) \mid \Sigma_1(R)$.*

Proof: By Theorem 2.8 and Lemma 2.2, $R[\Gamma_2 \cap \Gamma_1(R^{-1})] = \Gamma_2 \cap \Gamma_1(R) = \Gamma_2(R)$. Thus, $u = v = 1$ (see (2.5)). By Theorem 2.4, $\Sigma_1(R) = \frac{m}{t}\,\Sigma_2(R)$ and $t \mid m$, and this implies that $\Sigma_2(R) \mid \Sigma_1(R)$. ■

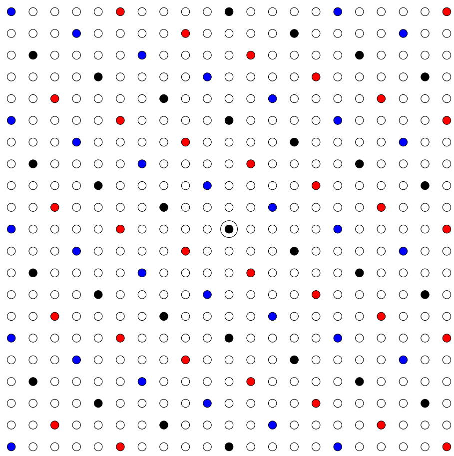
Corollary 2.11: *Let Γ_1 be a lattice having Γ_2 as a sublattice of index m. If $s = t = m$ in* (2.5)*, then $R \in OC(\Gamma_1)$ is a color coincidence of the coloring of Γ_1 induced by Γ_2 if and only if $\Sigma_2(R) = \Sigma_1(R)$.*

Proof: It follows from the previous proof that $\Sigma_2(R) = \Sigma_1(R)$ whenever R is a color coincidence of the coloring of Γ_1 with $t = m$. Conversely, if $\Sigma_2(R) = \Sigma_1(R)$ then $[\Gamma_1(R) : \Gamma_2(R)] = t \cdot u = s \cdot v = m$ and thus, $u = v = 1$. Hence, $R[\Gamma_2 \cap \Gamma_1(R^{-1})] = \Gamma_2(R) = \Gamma_2 \cap \Gamma_1(R)$, that is, R fixes color c_0. By Theorem 2.8, R must be a color coincidence of the coloring of Γ_1. ■

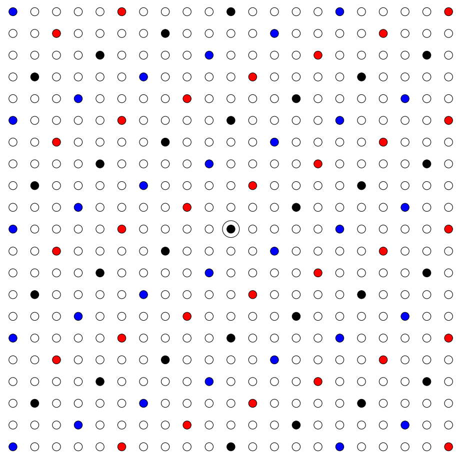
The condition $s = t = m$ in Corollary 2.11 means that all m colors of the coloring of Γ_1 are present in both colorings of $\Gamma_1(R^{-1})$ and $\Gamma_1(R)$ determined by Γ_2.

EXAMPLE 2.12: Take the rectangular sublattice $\Gamma_2 = \langle 3, i \rangle_{\mathbb{Z}}$ that is of index 3 in the square lattice $\Gamma_1 = \mathbb{Z}[i]$, and the coincidence rotation R in Example 2.6. Both colorings of $\Gamma_1(R^{-1})$ and $\Gamma_1(R)$ include three colors (see Figure 5), and thus, $s = t = 3$ in (2.5). Observe that R fixes the color black (corresponding to the coset $c_0 + \Gamma_2 = \Gamma_2$), which means that R is a color coincidence of the coloring of Γ_1 by Theorem 2.8.

Indeed, R fixes the color black, and interchanges the colors blue and red. Moreover, by Corollary 2.11, $\Sigma_2(R) = \Sigma_1(R)$. The CSL $\Gamma_2(R)$ is made up of all black dots in the coloring of $\Gamma_1(R)$.



(a) coloring of $\Gamma_1(R^{-1})$



(b) coloring of $\Gamma_1(R)$

FIGURE 5. The coincidence rotation R (the same as in Figure 4) is a color coincidence of the coloring of $\Gamma_1 = \mathbb{Z}[i]$ determined by the sublattice $\Gamma_2 = \langle 3, i \rangle_{\mathbb{Z}}$ because the color black (corresponding to Γ_2) is fixed by R. The blue and red colors are interchanged by R. The CSL $\Gamma_2(R)$ consists of all black dots in the coloring of $\Gamma_1(R)$.

For a given lattice Γ_1 and sublattice Γ_2 of Γ_1, denote by $\mathcal{H}$ the set of all color coincidences of the coloring of Γ_1 determined by Γ_2. Clearly, the identity isometry is in $\mathcal{H}$. In addition, it follows from the definition of a color coincidence that if $R \in \mathcal{H}$, then so is R^{-1}. The question of whether the product of two color coincidences is again a color coincidence, and in effect, whether $\mathcal{H}$ forms a group, is yet to be resolved. A step in answering this question is the following proposition.

Proposition 2.13: *Let Γ_2 be a sublattice of Γ_1 of index m, and $R_1, R_2 \in \mathcal{H}$. If $\Sigma_1(R_1)$ is relatively prime to $\Sigma_1(R_2)$, then $R_2R_1 \in \mathcal{H}$.*

Proof: Since $\Sigma_1(R_1)$ and $\Sigma_1(R_2)$ are relatively prime, $\Gamma_1(R_2R_1) = \Gamma_1 \cap R_2\Gamma_1 \cap R_2R_1\Gamma_1$ by Proposition 1.9(ii). Applying Theorem 2.8 and Lemma 2.2 to $R_1 \in \mathcal{H}$, one obtains $R_1\Gamma_2 \cap \Gamma_1 = R_1\Gamma_2 \cap \Gamma_1(R_1) = \Gamma_2 \cap \Gamma_1(R_1) = \Gamma_2 \cap R_1\Gamma_1$. Similarly, for $R_2 \in \mathcal{H}$, one has $R_2\Gamma_2 \cap \Gamma_1 = \Gamma_2 \cap R_2\Gamma_1$. It follows from these results that

$$\begin{aligned} R_2R_1\Gamma_2 \cap \Gamma_1(R_2R_1) &= R_2R_1\Gamma_2 \cap \Gamma_1 \cap R_2\Gamma_1 \\ &= R_2(R_1\Gamma_2 \cap \Gamma_1) \cap \Gamma_1 \\ &= R_2(\Gamma_2 \cap R_1\Gamma_1) \cap \Gamma_1 \\ &= (R_2\Gamma_2 \cap \Gamma_1) \cap R_2R_1\Gamma_1 \\ &= \Gamma_2 \cap R_2\Gamma_1 \cap R_2R_1\Gamma_1 \\ &= \Gamma_2 \cap \Gamma_1(R_2R_1). \end{aligned}$$

Thus, R_2R_1 fixes color $c_0 + \Gamma_2 = \Gamma_2$, which means that $R_2R_1 \in \mathcal{H}$ by Theorem 2.8. ■

2.3. Further examples

We are now going to implement the theory developed in the previous two sections to some special cases. Examples involving the cubic and hypercubic lattices are also presented in this section.

The next lemma considers the situation where at least one of the CSLs $\Gamma_1(R)$ and $\Gamma_1(R^{-1})$ lies in the sublattice Γ_2.

Lemma 2.14: *Let Γ_2 be a sublattice of Γ_1 with $[\Gamma_1 : \Gamma_2] = m$, and $R \in OC(\Gamma_1)$. If $\Gamma_1(R)$ or $\Gamma_1(R^{-1})$ is a sublattice of Γ_2, then $\Sigma_2(R) \mid \Sigma_1(R)$. In particular, both $\Gamma_1(R)$ and $\Gamma_1(R^{-1})$ are sublattices of Γ_2 if and only if $\Sigma_2(R) = \frac{1}{m}\Sigma_1(R)$.*

Proof: If $\Gamma_1(R)$ is a sublattice of Γ_2 then $\Gamma_2 \cap \Gamma_1(R) = \Gamma_1(R)$, that is, $t = 1$ in (2.5). Since $v \mid t$ by Theorem 2.4, $v = 1$. Equation (2.6) yields $\Sigma_1(R) = \frac{m}{s}\Sigma_2(R)$, and thus, $\Sigma_2(R) \mid \Sigma_1(R)$ because $s \mid m$.

Similarly, if Γ_2 contains $\Gamma_1(R^{-1})$ then $s = u = 1$. This, with (2.6), implies that $\Sigma_2(R) \mid \Sigma_1(R)$.

Finally, both $\Gamma_1(R)$ and $\Gamma_1(R^{-1})$ are sublattices of Γ_2 if and only if $s = t = u = v = 1$. Applying (2.6) completes the proof. ■

The possibilities are quite limited when the sublattice Γ_2 is of prime index in Γ_1, as can be seen in the next proposition.

Proposition 2.15: *Suppose Γ_2 is a sublattice of Γ_1 of index p, where p is prime, and $R \in OC(\Gamma_1)$.*

(i) *If both $\Gamma_1(R)$ and $\Gamma_1(R^{-1})$ are sublattices of Γ_2 then $\Sigma_2(R) = \frac{1}{p}\Sigma_1(R)$.*
(ii) *If either $\Gamma_1(R)$ or $\Gamma_1(R^{-1})$ is a sublattice of Γ_2 then $\Sigma_2(R) = \Sigma_1(R)$.*
(iii) *If neither $\Gamma_1(R)$ nor $\Gamma_1(R^{-1})$ is a sublattice of Γ_2, then $\Sigma_2(R) = \Sigma_1(R)$ whenever R is a color coincidence of the coloring of Γ_1 induced by Γ_2, and $\Sigma_2(R) = p\,\Sigma_1(R)$ otherwise.*

Proof: Statements (i) and (ii) are immediate from Lemma 2.14 and its proof.

If neither $\Gamma_1(R)$ nor $\Gamma_1(R^{-1})$ lie in Γ_2 then $s, t > 1$ (see (2.5)). Then, $s = t = p$ because both s and t divide the prime p by Theorem 2.4. Note that R is a color coincidence of the coloring of Γ_1 if and only if $u = v = 1$ by Theorem 2.8 and Lemma 2.2. Thus, $\Sigma_2(R) = \Sigma_1(R)$ whenever R is a color coincidence of the coloring of Γ_1 by (2.6). Otherwise, $u = v = p$ because $u \mid s$ and $v \mid t$, and it follows from (2.6) that $\Sigma_2(R) = p\,\Sigma_1(R)$. ■

The next proposition looks at the instance when the coincidence index of a coincidence isometry of a lattice Γ_1 is relatively prime to the index of the sublattice Γ_2 in Γ_1.

Proposition 2.16: *Let Γ_2 be a sublattice of Γ_1 with $[\Gamma_1 : \Gamma_2] = m$, and $R \in OC(\Gamma_1)$. If $\Sigma_1(R)$ and m are relatively prime, then all colors in the coloring of Γ_1 determined by Γ_2 appear in both colorings of $\Gamma_1(R)$ and $\Gamma_1(R^{-1})$, that is, $s = t = m$ in (2.5).*

Proof: From (2.6), $\frac{t}{m}\Sigma_1(R) = \frac{1}{u}\Sigma_2(R) \in \mathbb{N}$ because $u \mid \Sigma_2(R)$ (see Figure 2). Since $\Sigma_1(R)$ is relatively prime to m, $m \mid t$. However, $t \mid m$ as well by Theorem 2.4 and so $t = m$.

Similar arguments, where the second equality in (2.6) is used, yield $s = m$. ■

In the next two examples, we compute for the set of color coincidences $\mathcal{H}$ of colorings of cubic lattices. The cubic lattices are embedded in the Hurwitz ring $\mathbb{J}$ of integer quaternions and Cayley's parametrization of $SO(3,\mathbb{Q})$ is employed (see Subsections 1.2.3 and 1.2.4).

Example 2.17: Let Γ_1 be the body-centered cubic lattice $\Gamma_1 = \mathrm{Im}\,(\mathbb{J})$ and Γ_2 its maximal primitive cubic sublattice $\Gamma_2 = \mathrm{Im}\,(\mathbb{L})$. Here, $[\Gamma_1 : \Gamma_2] = 2$ and so the coloring of Γ_1 determined by Γ_2 consists of two colors. For each $R \in OC(\Gamma_1) = OC(\Gamma_2)$, one has $\Sigma_2(R) = \Sigma_1(R)$ (see Theorem 1.14).

Since all the coincidence indices of Γ_1 are odd numbers, both colorings of $\Gamma_1(R)$ and $\Gamma_1(R^{-1})$ induced by Γ_2 include two colors by Proposition 2.16. It follows then from Corollary 2.11 that all coincidence isometries of Γ_1 are color coincidences of the coloring of Γ_1 that fix both colors. Hence, $\mathcal{H}$ is the entire group $OC(\Gamma_1)$.

Example 2.18: Now, take the primitive cubic lattice $\Gamma_1 = \mathrm{Im}\,(\mathbb{L})$ to be the parent lattice and the body-centered cubic lattice $\Gamma_2 = 2\,\mathrm{Im}\,(\mathbb{J})$ to be the sublattice of Γ_1 of index 4. Write $\Gamma_1 = \bigcup_{j=0}^{3}(c_j + \Gamma_2)$ where $c_0 = 0$.

Arguments analogous to Example 2.17 yield that all four colors in the coloring of Γ_1 determined by Γ_2 show up in the coloring of $\Gamma_1(R)$ and $\Gamma_1(R^{-1})$, and $\mathcal{H} = OC(\Gamma_1)$.

Let $R = R_q \in SOC(\Gamma_1)$, where $q = (q_0, q_1, q_2, q_3)$ is a primitive quaternion. For sure, R is a color coincidence that fixes color c_0 because of Theorem 2.8. We shall now determine how R acts on the other colors c_1, c_2, c_3, and thus, the color permutation that R generates.

Since R is a color coincidence, it suffices to consider a representative from each coset of Γ_2 in Γ_1 that is in $\Gamma_1(R^{-1})$, and afterwards identify to which coset of Γ_2 the representative is sent by R. Take $c_1 = \Sigma_1(R)\mathbf{i}$, $c_2 = \Sigma_1(R)\mathbf{j}$, and $c_3 = \Sigma_1(R)\mathbf{k}$. Indeed, for $j \in \{1,2,3\}$, $c_j \notin \Gamma_2$ since $\Sigma_1(R)$ is odd, and $c_j \in \Gamma_1(R^{-1})$ because $\Sigma_1(R) = \mathrm{den}(R)$ ([**4**], see (1.5)). One obtains

$$R(c_1) = \tfrac{\Sigma_1(R)}{|q|^2}\, q\mathbf{i}\overline{q}\ ,\ R(c_2) = \tfrac{\Sigma_1(R)}{|q|^2}\, q\mathbf{j}\overline{q}\ ,\ R(c_3) = \tfrac{\Sigma_1(R)}{|q|^2}\, q\mathbf{k}\overline{q},$$

where $\frac{\Sigma_1(R)}{|q|^2} = \frac{1}{2^\ell}$ with $\ell \in \{0,1,2\}$. This gives rise to three different cases.

Before we proceed, we take note of the following lemmas that will be used in the computations thereafter.

Lemma 2.19: *The quaternion algebra* $\mathbb{H}$ *acts on* $\mathrm{Im}\,(\mathbb{H})$ *via* $qx\overline{q}$*, where* $q \in \mathbb{H}$ *and* $x \in \mathrm{Im}\,(\mathbb{H})$.

Lemma 2.20: *The sets*

$$(1,1,0,0)\mathbb{J} := \{(1,1,0,0)q : q \in \mathbb{J}\} = \left\{q \in \mathbb{J} : 2 \mid |q|^2\right\},$$
$$2\mathbb{J} := \{2q : q \in \mathbb{J}\} = \left\{q \in \mathbb{J} : 4 \mid |q|^2\right\}, \text{ and}$$
$$(1,1,0,0)2\mathbb{J} := \{(1,1,0,0)2q : q \in \mathbb{J}\} = \left\{q \in \mathbb{J} : 8 \mid |q|^2\right\}$$

are ideals of $\mathbb{J}$.

Proof: This is a consequence of Theorem 1.13. ∎

Lemma 2.21: *Let* $\Gamma_2 = 2\,\mathrm{Im}\,(\mathbb{J}) = 2\,\mathrm{Im}\,(\mathbb{L}) \cup [(0,1,1,1) + 2\,\mathrm{Im}\,(\mathbb{L})]$. *Then the following holds:*

(i) $2\mathbb{J} \cap \mathrm{Im}\,(\mathbb{H}) = 2\,\mathrm{Im}\,(\mathbb{L}) \subseteq \Gamma_2$
(ii) *If* $q \in \mathbb{J}$ *then* $q - \overline{q} \in \Gamma_2$.

Proof: Statement (i) is trivial. If $q \in \mathbb{L}$ then $q - \overline{q} \in 2\mathbb{J} \cap \mathrm{Im}\,(\mathbb{H}) \subseteq \Gamma_2$ by (i). On the other hand, if $q \in \mathbb{J} \setminus \mathbb{L}$ then $q - \overline{q} \in (0,1,1,1) + 2\,\mathrm{Im}\,(\mathbb{L}) \subseteq \Gamma_2$. This proves (ii). ∎

The three possible ratios of $\frac{\Sigma_1(R)}{|q|^2}$ are investigated below.

`Case I:` $\frac{\Sigma_1(R)}{|q|^2} = 1$, that is, $|q|^2 \equiv 1 \pmod 4$ and either one or three among the components of q is/are odd.

For instance, suppose q_0 is odd while q_1, q_2, q_3 are even, or q_0 is even while q_1, q_2, q_3 are odd. In both instances, one can write $q = r + s$, where $r \in 2\mathbb{J}$ and $s = \mathbf{e}$. One obtains

$$R(c_j) = qx_j\overline{q} = rx_j\overline{r} + rx_j\overline{s} + sx_j\overline{r} + sx_j\overline{s}$$

where $x_j = \mathbf{i},\mathbf{j},\mathbf{k}$ if $j = 1,2,3$, respectively. Lemmas 2.19, 2.20, and 2.21(i) imply that $rx_j\overline{r} \in \Gamma_2$, and $rx_j\overline{s} + sx_j\overline{r} = rx_j\overline{s} - \overline{rx_j\overline{s}} \in \Gamma_2$ by Lemma 2.21(ii). Hence, $R(c_j) \in sx_j\overline{s} + \Gamma_2 = x_j + \Gamma_2 = c_j + \Gamma_2$ for $j \in \{1,2,3\}$.

Similarly, for the other three possibilities, $R(c_j) \in c_j + \Gamma_2$ for $j \in \{1,2,3\}$ since for $s, x \in \{\mathbf{i},\mathbf{j},\mathbf{k}\}$, $sx\overline{s} = \begin{cases} x, & \text{if } s = x \\ -x, & \text{if } s \neq x. \end{cases}$ Therefore, in all instances, R fixes all colors.

`Case II:` $\frac{\Sigma_1(R)}{|q|^2} = \frac{1}{2}$, that is, $|q|^2 \equiv 2 \pmod 4$ and exactly two components of q are odd.

Consider the instance when both q_0 and q_1 are odd, or when both q_2 and q_3 are odd. Either way, one can express q as $q = r + s$ where $r \in 2\mathbb{J}$ and $s = (1,1,0,0)$. One has in this case

$$R(c_j) = \tfrac{1}{2}(rx_j\overline{r} + rx_j\overline{s} + sx_j\overline{r} + sx_j\overline{s})$$

where $x_j = \mathbf{i},\mathbf{j},\mathbf{k}$ if $j = 1,2,3$, respectively. Now, $\frac{1}{2}rx_j\overline{r} \in 2\mathbb{J}$ because 4 divides $\left|\frac{1}{2}rx_j\overline{r}\right|^2$. This, with Lemmas 2.19 and 2.21(i), implies that $\frac{1}{2}rx_j\overline{r} \in \Gamma_2$. Since $\frac{1}{2}rx_j\overline{s} \in \mathbb{J}$, one obtains that $\frac{1}{2}rx_j\overline{s} + \frac{1}{2}sx_j\overline{r} \in \Gamma_2$ by Lemma 2.21(ii). Therefore,

$$R(c_j) \in \tfrac{1}{2}sx_j\overline{s} + \Gamma_2 = \begin{cases} c_1 + \Gamma_2, & \text{if } j = 1 \\ c_3 + \Gamma_2, & \text{if } j = 2 \\ c_2 + \Gamma_2, & \text{if } j = 3. \end{cases}$$

Thus, R induces the permutation (c_2c_3) of colors. Similar computations for the other two possibilities (where one only needs to calculate the product $\frac{1}{2}sx\overline{s}$ for $s \in \{(1,0,1,0),(1,0,0,1)\}$ and $x \in \{\mathbf{i},\mathbf{j},\mathbf{k}\}$) yield that if q_0 and q_j are of the same parity, where $j \in \{1,2,3\}$, then R fixes both colors c_0 and c_j and swaps the other two colors.

`Case III:` $\frac{\Sigma_1(R)}{|q|^2} = \frac{1}{4}$, that is, $|q|^2 \equiv 0 \pmod 4$ and all components of q are odd.

Suppose an even number of components of q are congruent to 1 modulo 4. Then, one can write $q = r + s$, where $r \in (1,1,0,0)2\mathbb{J}$ and $s = (1,1,1,1)$. Thus,

$$R(c_j) = \tfrac{1}{4}(rx_j\overline{r} + rx_j\overline{s} + sx_j\overline{r} + sx_j\overline{s})$$

where $x_j = \mathbf{i},\mathbf{j},\mathbf{k}$ if $j = 1,2,3$, respectively. Since 4 divides $\left|\frac{1}{4}rx_j\overline{r}\right|^2$, one has $\frac{1}{4}rx_j\overline{r} \in 2\mathbb{J}$ and together with Lemmas 2.19 and 2.21(i), $\frac{1}{4}rx_j\overline{r} \in \Gamma_2$. Also, by Lemma 2.21(ii) one concludes that $\frac{1}{4}rx_j\overline{s} + \frac{1}{4}sx_j\overline{r} \in \Gamma_2$ because $\frac{1}{4}rx_j\overline{s} \in \mathbb{J}$. Finally,

$$R(c_j) \in \tfrac{1}{4}sx_j\overline{s} + \Gamma_2 = \begin{cases} c_2 + \Gamma_2, & \text{if } j = 1 \\ c_3 + \Gamma_2, & \text{if } j = 2 \\ c_1 + \Gamma_2, & \text{if } j = 3. \end{cases}$$

Hence, R generates the permutation $(c_1c_2c_3)$ of colors. On the other hand, if an odd number of components of q are congruent to 1 modulo 4, then similar arguments (where one only needs to compute for $\frac{1}{4}sx\overline{s}$ with $s = (1,1,1,-1)$ and $x \in \{\mathbf{i},\mathbf{j},\mathbf{k}\}$) show that R induces the permutation $(c_1c_3c_2)$ of colors.

Given a coincidence reflection $T_q \in OC(\Gamma_1)$, the color permutation that it effects is the same as that of the coincidence rotation R_q. This follows from the fact that $\Sigma_1(T_q) = \Sigma_1(R_q)$ and from the following choice of coset representatives: $c_1 = -\Sigma_1(R_q)\mathbf{i}$, $c_2 = -\Sigma_1(R_q)\mathbf{j}$, and $c_3 = -\Sigma_1(R_q)\mathbf{k}$.

In conclusion, if a coincidence isometry $R \in OC(\Gamma_1)$ is parametrized by the primitive quaternion q, then

(i) R fixes all the colors if and only if $|q|^2 \equiv 1 \pmod 4$,
(ii) R fixes two of the colors (one of the fixed colors is c_0) if and only if $|q|^2 \equiv 2 \pmod 4$, and
(iii) R fixes only color c_0 if and only if $|q|^2 \equiv 0 \pmod 4$.

Moreover, the set of color permutations generated by the color coincidences of the coloring of Γ_1 forms a group that is isomorphic to S_3.

The following example examines the set of color coincidences $\mathcal{H}$ of the coloring of D_4 determined by $\mathbb{Z}^4$. In this case, $\mathcal{H}$ forms a proper subgroup of $OC(D_4) = O(4,\mathbb{Q})$. In the process, a simpler formula giving the coincidence index of an $R \in OC(\mathbb{Z}^4)$ that does not involve $\mathrm{den}(R)$ arises (see (1.6)). As before, D_4 and $\mathbb{Z}^4$ are identified with the set of Hurwitz quaternions $\mathbb{J}$ and the set of Lipschitz quaternions $\mathbb{L}$, respectively. Also, coincidence isometries of D_4 (and $\mathbb{Z}^4$) are parametrized by admissible pairs of primitive quaternions (refer to Chapters 1.2.3 and 1.2.5).

Example 2.22: Take Γ_1 to be the centered hypercubic lattice $\Gamma_1 = \mathbb{J}$ and Γ_2 to be the primitive hypercubic lattice $\Gamma_2 = \mathbb{L}$ of index 2 in Γ_1. Let $R = R_{q,p} \in SOC(\Gamma_1)$ be parametrized by the admissible pair (q,p) of primitive quaternions.

Since $[\Gamma_1 : \Gamma_2] = 2$ and $\Sigma_1(R)$ is always odd, $s = t = 2$ by Proposition 2.16. It follows then from Theorem 2.4 that $\Sigma_2(R) = u\,\Sigma_1(R)$ with $u = 1$ or $u = 2$. In particular, $\Sigma_2(R) = \Sigma_1(R)$ if and only if $R \in \mathcal{H}$ by Corollary 2.11. The following looks at the conditions that the quaternion pair (q,p) should satisfy so that $R \in \mathcal{H}$.

Going through the different possible admissible quaternion pairs (q,p) results in the following cases. In each case, the sets $R\Gamma_2 \cap \Gamma_1(R)$ and $\Gamma_2 \cap \Gamma_1(R)$ are compared in order to ascertain whether $R \in \mathcal{H}$ or not (see Theorem 2.8).

`Case I:` $|q|^2$ and $|p|^2$ are odd

Suppose $v \in \Gamma_2 \cap \Gamma_1(R)$ and write $v = \frac{qw\overline{p}}{|q\,\overline{p}|}$ for some $w \in \mathbb{J}$. This means that $|q\,\overline{p}|\,v = qw\overline{p} \in \mathbb{L}$. Since $|q|^2$ and $|p|^2$ are odd, one can express $q = r_1 + s_1$ and $p = r_2 + s_2$, where $r_1, r_2 \in 2\mathbb{J}$, and $s_1, s_2 \in \{\mathbf{e}, \mathbf{i}, \mathbf{j}, \mathbf{k}\}$. With this, one obtains

$$qw\overline{p} = r_1 w\overline{r_2} + r_1 w\overline{s_2} + s_1 w\overline{r_2} + s_1 w\overline{s_2} \in \mathbb{L}.$$

By Lemma 2.20, $r_1 w\overline{r_2} + r_1 w\overline{s_2} + s_1 w\overline{r_2} \in 2\mathbb{J} \subseteq \mathbb{L}$, which implies that $s_1 w\overline{s}_2 \in \mathbb{L}$ and hence, $w \in \mathbb{L}$. Thus, $v = Rw \in R\Gamma_2$ and $\Gamma_2 \cap \Gamma_1(R) \subseteq R\Gamma_2 \cap \Gamma_1(R)$. It follows then that $R\Gamma_2 \cap \Gamma_1(R) = \Gamma_2 \cap \Gamma_1(R)$ because $s = t = 2$, and so $R \in \mathcal{H}$.

`Case II:` $|q|^2$ is odd and $|p|^2 \equiv 0 \pmod 4$, or $|q|^2 \equiv 0 \pmod 4$ and $|p|^2$ is odd

Consider $x = \frac{1}{2}\,|q\,\overline{p}| \in \mathbb{L}$. One has $R(x) = \frac{qx\overline{p}}{|q\,\overline{p}|} = \frac{1}{2}q\,\overline{p} \in \mathbb{J}$. Thus, $R(x) \in R\Gamma_2 \cap \Gamma_1(R)$. However, the first component of $q\,\overline{p}$, which is equal to $\langle q, p\rangle$, is odd. This implies that $\frac{1}{2}q\,\overline{p} \notin \mathbb{L}$ and $R(x) \notin \Gamma_2 \cap \Gamma_1(R)$. Hence, $R\Gamma_2 \cap \Gamma_1(R) \neq \Gamma_2 \cap \Gamma_1(R)$ and $R \notin \mathcal{H}$.

`Case III:` $|q|^2 \equiv |p|^2 \equiv 2 \pmod 4$

Write $q = r_1 + s_1$ and $p = r_2 + s_2$ where r_1, $r_2 \in 2\mathbb{J}$ and

$$s_1, s_2 \in \{(1,1,0,0), (1,0,1,0), (1,0,0,1)\}.$$

Note that $\langle q, p\rangle$ is even if and only if $s_1 = s_2$.

Consider again $x = \frac{1}{2}\,|q\,\overline{p}| \in \mathbb{L}$ so that $R(x) = \frac{1}{2}q\,\overline{p} \in R\Gamma_2 \cap \Gamma_1(R)$. Now, $\frac{1}{2}q\,\overline{p} \notin \mathbb{L}$ if and only if $\langle q, p\rangle$ is odd. Since $\frac{1}{2}q\,\overline{p} \notin \mathbb{L}$ implies that $R\Gamma_2 \cap \Gamma_1(R) \neq \Gamma_2 \cap \Gamma_1(R)$, $R \notin \mathcal{H}$ whenever $\langle q, p\rangle$ is odd.

It remains to check the case $s_1 = s_2$. Take $v \in \Gamma_2 \cap \Gamma_1(R)$. Write $v = \frac{qw\overline{p}}{|q\,\overline{p}|}$ for some $w \in \mathbb{J}$. One has

$$\tfrac{1}{2}\,|q\,\overline{p}|\,v = \tfrac{1}{2}(r_1 w\overline{r_2} + r_1 w\overline{s_1} + s_1 w\overline{r_2} + s_1 w\overline{s_1}) \in \mathbb{L}.$$

Now, $\frac{1}{2}r_1 w\overline{r_2} \in 2\mathbb{J} \subseteq \mathbb{L}$ and $\frac{1}{2}r_1 w\overline{s_1}$, $\frac{1}{2}s_1 w\overline{r_2} \in (1,1,0,0)\mathbb{J} \subseteq \mathbb{L}$ by Lemma 2.20. Hence, $\frac{1}{2}s_1 w\overline{s_1} = s_1 w {s_1}^{-1} \in \mathbb{L}$ meaning $w \in {s_1}^{-1}\mathbb{L}s_1 = \mathbb{L}$ for all three possible values of s_1. It follows then that $v \in R\Gamma_2$ and $R\Gamma_2 \cap \Gamma_1(R) = \Gamma_2 \cap \Gamma_1(R)$. Thus, $R \in \mathcal{H}$ if $\langle q, p\rangle$ is even.

`Case IV:` $|q|^2 \equiv |p|^2 \equiv 0 \pmod 4$

Write $q = r_1 + s_1$ and $p = r_2 + s_2$ where $r_1, r_2 \in (1,1,0,0)2\mathbb{J}$ and

$$s_1, s_2 \in \{(1,1,1,1), (1,1,1,-1)\}.$$

Note that $4 \mid \langle q, p\rangle$ if and only if $s_1 = s_2$.

Take $x = \frac{1}{4}\left|q\,\overline{p}\right| \in \mathbb{L}$. One obtains $R(x) = \frac{1}{4}q\,\overline{p} = \left(\frac{1}{2}q\right)\left(\frac{1}{2}\overline{p}\right) \in \mathbb{J}$. Hence, $Rx \in R\Gamma_2 \cap \Gamma_1(R)$. Observe however that $\frac{1}{4}q\,\overline{p} \notin \mathbb{L}$ if and only if $4 \nmid \langle q,p\rangle$. Since $\frac{1}{4}q\,\overline{p} \notin \mathbb{L}$ means that $R\Gamma_2 \cap \Gamma_1(R) \neq \Gamma_2 \cap \Gamma_1(R)$, $4 \nmid \langle q,p\rangle$ implies $R \notin \mathcal{H}$.

Again, it remains to check the instance when $s_1 = s_2$. Let $v \in \Gamma_2 \cap \Gamma_1(R)$. If one writes $v = \frac{qw\overline{p}}{|q\,\overline{p}|}$ for some $w \in \mathbb{J}$, one gets

$$\tfrac{1}{4}\left|q\,\overline{p}\right| v = \tfrac{1}{4}(r_1 w\overline{r_2} + r_1 w\overline{s_1} + s_1 w\overline{r_2} + s_1 w\overline{s_1}) \in \mathbb{L}.$$

By Lemma 2.20, $\frac{1}{4}r_1 w\overline{r_2}$, $\frac{1}{4}r_1 w\overline{s_1}$, and $\frac{1}{4}s_1 w\overline{r_2} \in (1,1,0,0)\mathbb{J} \subseteq \mathbb{L}$. Therefore, $\frac{1}{4}s_1 w\overline{s_1} = s_1 w {s_1}^{-1} \in \mathbb{L}$ or $w \in {s_1}^{-1}\mathbb{L}s_1 = \mathbb{L}$ for both possible values of s_1. Hence, $v \in R\Gamma_2$ which implies that $R\Gamma_2 \cap \Gamma_1(R) = \Gamma_2 \cap \Gamma_1(R)$. Therefore, $R \in \mathcal{H}$ whenever $\langle q,p\rangle$ is divisible by 4.

The results above also hold for coincidence reflections $T_{q,p} = R_{q,p} \cdot T_{1,1} \in OC(\Gamma_1)$ since $\Sigma_1(T_{q,p}) = \Sigma_1(R_{q,p})$, $\overline{w} \in \mathbb{L}$ if and only if $w \in \mathbb{L}$, and $\overline{x} = x$ when $\mathrm{Im}\,(x) = 0$.

We now show that $\mathcal{H}$ in this instance forms a group. From above, one sees that $\mathcal{H} = \{R \in OC(\Gamma_1) : \Sigma_2(R) = \Sigma_1(R)\}$. Moreover, because either $\Sigma_2(R) = \Sigma_1(R)$ or $\Sigma_2(R) = 2\,\Sigma_1(R)$, and $\Sigma_1(R)$ is odd for all $R \in OC(\Gamma_1)$, one can write $\mathcal{H} = \{R \in OC(\Gamma_1) : \Sigma_2(R) \text{ is odd}\}$. Now, if $R_1, R_2 \in \mathcal{H}$ then $\Sigma_2(R_2R_1) \mid \Sigma_2(R_2) \cdot \Sigma_2(R_1)$ by Proposition 1.9(i). This implies that $\Sigma_2(R_2R_1)$ must also be odd, and hence $R_2R_1 \in \mathcal{H}$. This proves that the product of two color coincidences of the coloring of Γ_1 is again in $\mathcal{H}$, and hence, $\mathcal{H}$ is a subgroup of $OC(\Gamma_1)$.

Finally, all of these yield the following result about the coincidence index of a coincidence isometry of $\mathbb{Z}^4$ (compare with (1.6)).

Proposition 2.23: *Let $R_{q,p} \in SOC(\mathbb{Z}^4)$ where (q,p) is an admissible pair of primitive quaternions. Then either*

$$\Sigma_{\mathbb{Z}^4}(R_{q,p}) = \Sigma_{D_4}(R_{q,p}) = \mathrm{lcm}\left(\tfrac{|q|^2}{2^k}, \tfrac{|p|^2}{2^\ell}\right) \quad \textit{or} \;\; \Sigma_{\mathbb{Z}^4}(R_{q,p}) = 2\Sigma_{D_4}(R_{q,p}),$$

where k and ℓ are the highest powers such that 2^k and 2^ℓ divide $|q|^2$ and $|p|^2$, respectively. In particular, $\Sigma_{\mathbb{Z}^4}(R_{q,p}) = \Sigma_{D_4}(R_{q,p})$ holds if and only if one of the following conditions are satisfied:

(i) $|q|^2$ *and* $|p|^2$ *are odd,*
(ii) $|q|^2 \equiv |p|^2 \equiv 2 \pmod 4$ *with* $\langle q,p\rangle$ *even,*
(iii) $|q|^2 \equiv |p|^2 \equiv 0 \pmod 4$ *with* $4 \mid \langle q,p\rangle$.

The same holds for $T_{q,p} \in OC(\mathbb{Z}^4) \setminus SOC(\mathbb{Z}^4)$.

Note that Proposition 2.23 is consistent and similar to the conditions set forth in [**82**] on how to identify which of the 576 pure symmetry rotations of D_4 are also pure symmetry rotations of $\mathbb{Z}^4$.

2.4. Application to quasicrystals

Even though the results in this chapter were explicitly stated for lattices, they also hold for $\mathbb{Z}$-modules in $\mathbb{R}^d$ (see Remark 1.10). This suggests that the same techniques are applicable when dealing with quasicrystals. In fact, the coincidence problem for the set of vertex points of a quasicrystalline tiling breaks into two parts: the coincidence problem for the underlying limit translation module, and the computation of the window correction factor [**59, 4**]. The latter depends on the geometry of the window and is equal to 1 if the window is circular. In such a case, results for the underlying module are exactly the same as that for the set of vertex points of the tiling. We illustrate with the following example how the results in this chapter are adapted to the quasicrystal setting.

EXAMPLE 2.24: Consider the set of vertex points P_1 of the eightfold symmetric Ammann-Beenker tiling (see Figure 6). Here, one needs to consider the coincidence problem for the underlying module M_1 which is the standard eightfold planar module $\mathcal{M}_8 = \mathbb{Z}[\xi]$ of rank 4, where $\xi = \xi_8 = e^{\pi i/4}$ (refer to Chapter 1.2.2). That is, P_1 is treated as a discrete subset of M_1 embedded in the complex plane. Even though the discussion of the window correction factor is omitted here, notice that the acceptance factor for the Ammann-Beenker tiling is anyway very close to 1 [**59**].

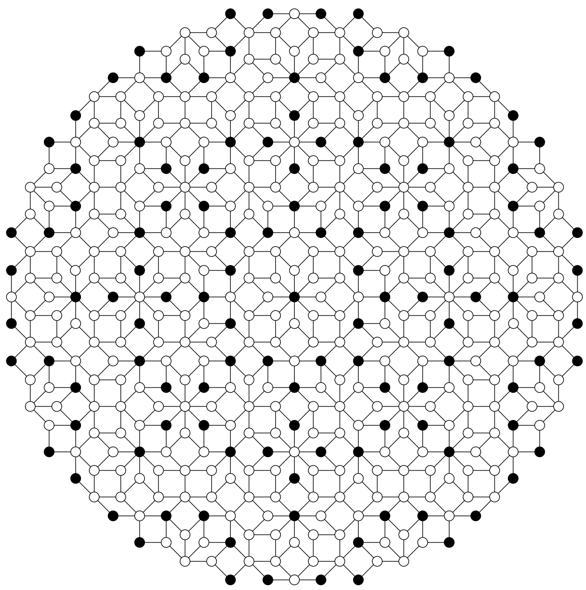
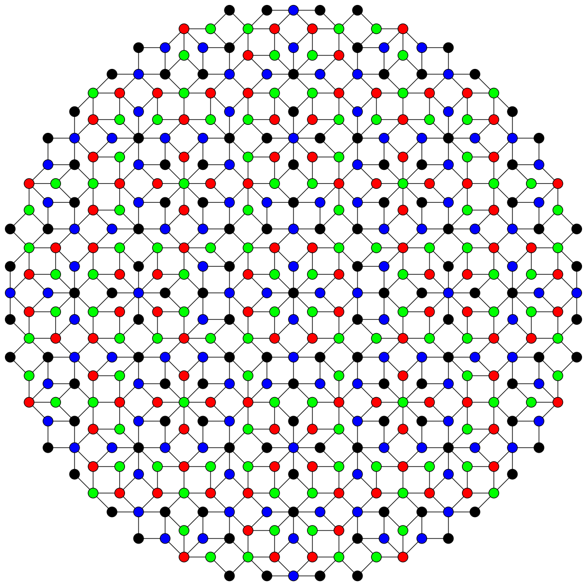


FIGURE 6. The set of vertices P_1 of the Ammann-Beenker tiling and the subset P_2 (colored black) of P_1

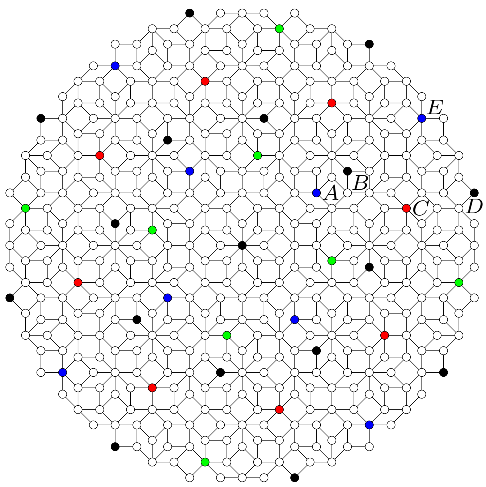
Let P_2 be the set of points of P_1 colored black in Figure 6. The subset P_2 can be obtained as the intersection of the submodule $M_2 = \langle 1 + \xi^2 \rangle$ (of index 4 in M_1) and P_1. Choose the coincidence rotation $R = R_{1+\xi+\xi^3,1}$ of M_1 (and P_1) (see Remark 1.12) which corresponds to the counterclockwise rotation about the origin at an angle of $\tan^{-1}\left(-2\sqrt{2}\right) \approx 109.5°$. The coincidence index of R with respect to M_1 is 9.

A coloring of P_1 with four colors determined by P_2 is shown in Figure 7(a) (see also [**16**, Fig. 1]). Denote by $P_1(R^{-1})$ and $P_1(R)$ the set of coinciding points of P_1 and $R^{-1}P_1$, and of P_1 and RP_1, respectively. Figures 7(b) and 7(c) show the colorings of $P_1(R^{-1})$ and $P_1(R)$ induced by the coloring of P_1. Observe that all four colors appear in both colorings. Since M_1 and M_2 are similar modules, the coincidence index of R with respect to M_2 is also 9 by Theorem 1.3 (applied to similarity modules). Hence,

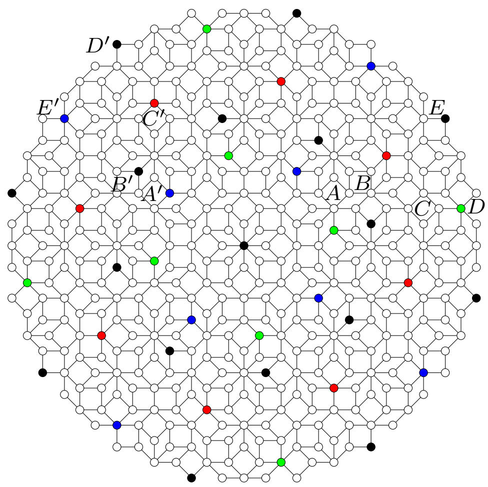
R is a color coincidence of the coloring (with all colors being fixed), and the set of coinciding points, $P_2(R)$, includes all points of P_2 in the coloring of $P_1(R)$.



(a) Coloring of P_1 determined by P_2



(b) Coloring of $P_1(R^{-1})$



(c) Coloring of $P_1(R)$

FIGURE 7. Colorings of $P_1(R^{-1})$ and $P_1(R)$ determined by P_2 (see Figure 6), where the coincidence rotation R corresponds to a rotation about the origin by $\tan^{-1}\left(-2\sqrt{2}\right) \approx 109.5°$ in the counterclockwise direction. The points labeled A, B, C, D, and E are mapped by R to the points labeled A', B', C', D', and E', respectively. R is a color coincidence of the coloring of P_1 that fixes all the colors. The intersection of P_2 and RP_2, $P_2(R)$, is made up of all black dots in the coloring of $P_1(R)$.

CHAPTER 3

Coincidences of shifted lattices

The chapter starts with an investigation of how points on a lattice and points on the image of the lattice under a general (affine) isometry may coincide. A closely related subject, and the main topic of this chapter, is subsequently discussed: the coincidence problem for shifted lattices. That is, upon translating the lattice by some vector and afterwards applying a linear isometry on the shifted lattice (with respect to the origin), its intersection (if any) with the shifted lattice is considered. An extensive analysis of the coincidences of a shifted square lattice follows the general discussion. Remarks on how general results for lattices extend to $\mathbb{Z}$-modules, as well as several results on the coincidences of shifted planar modules based on the solution of the coincidence problem for a shifted square lattice, conclude the chapter.

3.1. Affine coincidences

Let $\Gamma \subseteq \mathbb{R}^d$ be a lattice. A subset of Γ will be called a *cosublattice of* Γ if it is a coset of some sublattice Γ' of Γ. One can think of a cosublattice of Γ as a shifted copy of Γ' by some vector of Γ. Since all cosets of a group have the same order by Langrange's Theorem, the *index of a cosublattice* $\ell + \Gamma'$ *of* Γ, denoted by $[\Gamma : \ell + \Gamma']$, is defined as the (group) index of the sublattice Γ' in Γ, that is, $[\Gamma : \ell + \Gamma'] = [\Gamma : \Gamma'] < \infty$. This definition of index makes sense geometrically for lattices (as oppose to $\mathbb{Z}$-modules): a translation does not change the volume of fundamental domains of Γ and Γ', and so $[\Gamma : \Gamma'] = [\ell + \Gamma : \ell + \Gamma'] = [\Gamma : \ell + \Gamma']$.

Denote by $E(d)$ the group of isometries of $\mathbb{R}^d$. An $f \in E(d)$ shall be written as $f = (v, R)$, where $f : x \mapsto v + R(x)$, with $R \in O(d)$ (the linear part of f) and $v \in \mathbb{R}^d$ (the translational part of f). The next definition generalizes the concept of a linear coincidence isometry to an affine coincidence isometry.

Definition 3.1: Let Γ be a lattice in $\mathbb{R}^d$ and $f \in E(d)$. Then f is an *affine coincidence isometry* of Γ if $\Gamma \cap f\Gamma$ contains a cosublattice of Γ.

The set of affine coincidence isometries of Γ shall be denoted by $AC(\Gamma)$. Clearly, $AC(\Gamma)$ contains the symmetry group of Γ and the group $OC(\Gamma) = AC(\Gamma) \cap O(d) = \{(v, R) \in AC(\Gamma) : v = 0\}$.

The following lemma describes the intersection of two lattices that are related by some isometry.

Lemma 3.2: *Let* $\Gamma \in \mathbb{R}^d$ *be a lattice and* $(v, R) \in E(d)$*. If* $v \in \ell + R\Gamma$ *for some* $\ell \in \Gamma$*, then* $\Gamma \cap (v, R)\Gamma = \ell + (\Gamma \cap R\Gamma)$.

Proof: Since $v \in \ell + R\Gamma$, $(v, R)\Gamma = (\ell, R)\Gamma$ and so $\Gamma \cap (v, R)\Gamma = \Gamma \cap (\ell, R)\Gamma$. It remains to show that $\Gamma \cap (\ell, R)\Gamma = \ell + (\Gamma \cap R\Gamma)$.

Take $x \in \Gamma \cap (\ell, R)\Gamma$ and write $x = \ell + R\ell'$ for some $\ell' \in \Gamma$. Then $x \in \ell + (\Gamma \cap R\Gamma)$ because $R\ell' = x - \ell \in \Gamma \cap R\Gamma$. The opposite inclusion is clear. ■

Lemma 3.2 brings about the following characterization of an affine coincidence isometry of a lattice.

Theorem 3.3: *Let Γ be a lattice in $\mathbb{R}^d$. Then $(v, R) \in E(d)$ is an affine coincidence isometry of Γ if and only if $R \in OC(\Gamma)$ and $v \in \Gamma + R\Gamma$.*

Proof: It follows from Lemma 3.2 that if $R \in OC(\Gamma)$ and $v \in \Gamma + R\Gamma$ then $\Gamma \cap (v, R)\Gamma$ is a coset of the CSL $\Gamma(R)$. Hence, $(v, R) \in AC(\Gamma)$.

In the other direction, let $(v, R) \in AC(\Gamma)$. Because $\Gamma \cap (v, R)\Gamma \neq \varnothing$, there exist $\ell, \ell' \in \Gamma$ with $\ell = v + R\ell'$, and so $v = \ell - R\ell' \in \ell + R\Gamma \subseteq \Gamma + R\Gamma$. By Lemma 3.2, one obtains $\Gamma \cap (v, R)\Gamma = \ell + (\Gamma \cap R\Gamma)$. Thus,

$$[\Gamma : \Gamma \cap R\Gamma] = [\Gamma : \ell + (\Gamma \cap R\Gamma)] = [\Gamma : \Gamma \cap (v, R)\Gamma] < \infty,$$

which means that $\Gamma \cap R\Gamma$ is a sublattice of Γ. Therefore, Γ is commensurate to $R\Gamma$, and $R \in OC(\Gamma)$. ■

The set of affine coincidences of a lattice $\Gamma \subseteq \mathbb{R}^d$ is now given by

$$AC(\Gamma) = \{(v, R) \in E(d) : R \in OC(\Gamma) \text{ and } v \in \Gamma + R\Gamma\}.$$

Moreover, if $(v, R) \in AC(\Gamma)$ with $v \in \ell + R\Gamma$ for some $\ell \in \Gamma$, then

$$\Gamma \cap (v, R)\Gamma = \ell + \Gamma(R) \tag{3.1}$$

by Lemma 3.2. Thus, $\Gamma \cap (v, R)\Gamma$ is a coset of the CSL $\Gamma(R)$. This means that the intersection $\Gamma \cap (v, R)\Gamma$ does not only contain a cosublattice of Γ but is in fact a cosublattice of Γ. For this reason, we shall refer to $\Gamma \cap (v, R)\Gamma$ as an *affine coincidence site lattice* (ACSL) of Γ. In addition, each $R \in OC(\Gamma)$ corresponds to $\Sigma(R) = [\Gamma : \Gamma(R)]$ distinct possible ACSLs.

REMARK 3.4: Another lattice of interest in the study of grain boundaries is the so-called *displacement shift complete* (DSC) *lattice*. It is the lattice formed by all possible displacement vectors that preserve the structure of the grain boundary. In this setting, given a linear coincidence isometry R of the lattice Γ, the corresponding DSC lattice is $\{v : (v, R) \in AC(\Gamma)\} = \Gamma + R\Gamma$ by Theorem 3.3. This conclusion is in agreement with the main result of [**35**], which states that the DSC lattice formed by Γ and $R\Gamma$ is the dual lattice of the CSL formed by Γ^* and $(R\Gamma)^*$, that is, $[\Gamma^* \cap (R\Gamma)^*]^* = \Gamma + R\Gamma$.

Observe that the identity isometry $\mathbb{1}_d \in AC(\Gamma)$ for any lattice Γ in $\mathbb{R}^d$. In addition, the inverse of every isometry in $AC(\Gamma)$ is also in $AC(\Gamma)$. Indeed, if $(v, R) \in AC(\Gamma)$, then it follows from Theorem 3.3 that $(v, R)^{-1} = (-R^{-1}v, R^{-1}) \in AC(\Gamma)$ since $R^{-1} \in OC(\Gamma)$ and $-R^{-1}v \in \Gamma + R^{-1}\Gamma$. However, the product of two affine coincidence isometries of Γ may or may not be an element of $AC(\Gamma)$. Thus, the set $AC(\Gamma)$ does not always form a group. The next proposition tells us exactly when $AC(\Gamma)$ is a group.

Proposition 3.5: *Let $\Gamma \subseteq \mathbb{R}^d$ be a lattice. Then $AC(\Gamma)$ is a group if and only if it is the symmetry group G of Γ.*

Proof: Suppose $AC(\Gamma)$ is a group and take $(v, R) \in AC(\Gamma)$. By Theorem 3.3, $R \in OC(\Gamma)$, and thus, $(0, R^{-1}) = R^{-1} \in OC(\Gamma) \subseteq AC(\Gamma)$. Seeing that $AC(\Gamma)$ is a group, the product $(v, R)(0, R^{-1}) = (v, \mathbb{1}_d) \in AC(\Gamma)$. It follows then from Theorem 3.3 that $v \in \Gamma$. Furthermore, $\Gamma + R\Gamma = \Gamma$, for if $w \in \Gamma + R\Gamma$ then $(w, R) \in AC(\Gamma)$, and so $w \in \Gamma$. Hence, $R \in P(\Gamma)$. Since G is symmorphic, that is, G is the semidirect product of $P(\Gamma)$ with its translation subgroup $T(G) = \Gamma$, one obtains $(v, R) \in G$. ■

3.2. The coincidence problem for a shifted lattice

We now turn our attention to lattices Γ in $\mathbb{R}^d$ that are shifted by some vector $x \in \mathbb{R}^d$. By a *cosublattice of the shifted lattice* $x + \Gamma$, we mean a subset of $x + \Gamma$ of the form $x + \Gamma'$ where Γ' is a cosublattice of Γ. In addition, the *index of the cosublattice* $x + \Gamma'$ *in* $x + \Gamma$ is understood to be $[x + \Gamma : x + \Gamma'] := [\Gamma : \Gamma']$. There is no ambiguity here - relabeling x as the origin gives back the original lattice Γ. Of particular interest in this section, and the remainder of the chapter, are intersections of the form $(x + \Gamma) \cap R(x + \Gamma)$, where $R \in O(d)$.

Definition 3.6: An $R \in O(d)$ is said to be a (*linear*) *coincidence isometry of the shifted lattice* $x + \Gamma$ if $(x + \Gamma) \cap R(x + \Gamma)$ is a cosublattice of $x + \Gamma$.

The intersection $(x+\Gamma) \cap R(x+\Gamma)$ will also be referred to as a CSL of the shifted lattice $x + \Gamma$, while the coincidence index of R with respect to $x + \Gamma$ is taken to be $\Sigma_{x+\Gamma}(R) := [x + \Gamma : (x + \Gamma) \cap R(x + \Gamma)]$. The set of all coincidence isometries of $x + \Gamma$ shall be denoted by $OC(x+\Gamma)$. Likewise, we take $SOC(x+\Gamma) := OC(x+\Gamma) \cap SO(d)$.

Remark 3.7: Observe that applying a linear isometry R on the shifted lattice $x + \Gamma$ is equivalent to applying the same isometry R but with center at $-x$ on the original lattice Γ. Hence, just as $OC(\Gamma)$ is an extension of $P(\Gamma)$, one may interpret $OC(x+\Gamma)$ as a generalization of the site-symmetry group of the point $-x$.

We now aim to characterize a coincidence isometry R of $x + \Gamma$ and identify the CSL of $x + \Gamma$ generated by R. To do this, write $(x + \Gamma) \cap R(x + \Gamma)$ as

$$(x + \Gamma) \cap R(x + \Gamma) = (x, \mathbb{1}_d)\Gamma \cap (Rx, R)\Gamma = (x, \mathbb{1}_d)[\Gamma \cap (Rx - x, R)\Gamma]. \tag{3.2}$$

That is, $(x + \Gamma) \cap R(x + \Gamma)$ may be obtained by shifting $\Gamma \cap (Rx - x, R)\Gamma$ by x. This means that $(x+\Gamma) \cap R(x+\Gamma)$ is a cosublattice of $x+\Gamma$ if and only if $\Gamma \cap (Rx-x, R)\Gamma$ is a cosublattice of Γ, which is equivalent to saying that $(Rx - x, R) \in AC(\Gamma)$. It now follows from Theorem 3.3 that $R \in OC(x + \Gamma)$ if and only if $R \in OC(\Gamma)$ and $Rx - x \in \Gamma + R\Gamma$. Furthermore, the CSL $(x+\Gamma) \cap R(x+\Gamma)$ of $x+\Gamma$ can be expressed as a shifted copy of the CSL $\Gamma(R)$ of Γ by applying (3.1) to (3.2). All of these constitute the proof of the following theorem.

Theorem 3.8: *Let* Γ *be a lattice in* $\mathbb{R}^d$ *and* $x \in \mathbb{R}^d$. *Then*

$$OC(x + \Gamma) = \{R \in OC(\Gamma) : Rx - x \in \Gamma + R\Gamma\}.$$

In addition, if $R \in OC(x + \Gamma)$ *with* $Rx - x \in \ell + R\Gamma$ *for some* $\ell \in \Gamma$, *then*

$$(x + \Gamma) \cap R(x + \Gamma) = (x + \ell) + \Gamma(R). \tag{3.3}$$

Equation (3.3) indicates that the CSL of $x+\Gamma$ obtained from $R \in OC(x+\Gamma)$ is just a translate of some coset of the CSL $\Gamma(R)$ in Γ by x. Consequently,

$$\Sigma_{x+\Gamma}(R) = \Sigma_\Gamma(R) \tag{3.4}$$

for all $R \in OC(x+\Gamma)$. This means that shifting a lattice does not yield any new values of coincidence indices.

Let $S \in P(\Gamma)$. If $R \in OC(\Gamma)$ then $RS \in OC(\Gamma)$ and the CSLs generated by R and RS are the same, that is, $\Gamma(RS) = \Gamma(R)$. However, the corresponding statement for coincidence isometries of a shifted lattice does not always hold, as can be seen in the next proposition.

Proposition 3.9: *Let $\Gamma \subseteq \mathbb{R}^d$ be a lattice and $x \in \mathbb{R}^d$, and suppose that $R, RS \in OC(x+\Gamma)$ with $S \in P(\Gamma)$. Then $(x+\Gamma) \cap RS(x+\Gamma) = (x+\Gamma) \cap R(x+\Gamma)$ if and only if $Sx - x \in \Gamma$.*

Proof: It follows from Theorem 3.8 that

$$Rx - x \in \ell_1 + R\Gamma \text{ and } RSx - x \in \ell_2 + RS\Gamma = \ell_2 + R\Gamma$$

for some $\ell_1, \ell_2 \in \Gamma$. In addition, (3.3) yields

$$(x+\Gamma) \cap RS(x+\Gamma) = \ell_1 + \Gamma(RS) = \ell_1 + \Gamma(R) \text{ and } (x+\Gamma) \cap R(x+\Gamma) = \ell_2 + \Gamma(R).$$

Hence, $(x+\Gamma) \cap RS(x+\Gamma) = (x+\Gamma) \cap R(x+\Gamma)$ if and only if $\ell_2 - \ell_1 \in R\Gamma$. Now, $R(Sx - x) = RSx - Rx \in (\ell_2 - \ell_1) + R\Gamma$. This implies that $\ell_2 - \ell_1 \in R\Gamma$ if and only if $Sx - x \in \Gamma$, which proves the claim. ■

Proposition 3.9 will prove to be useful when counting the number of CSLs of a shifted lattice of a given index.

For a given lattice $\Gamma \subseteq \mathbb{R}^d$, it is enough to consider values of x in a fundamental domain of Γ to compute for all the different possible sets $OC(x+\Gamma)$, because $OC(x+\Gamma) = OC[(x+\ell)+\Gamma]$ for all $\ell \in \Gamma$. The next proposition asserts even more; it suffices to look at values of x in a fundamental domain of the symmetry group of Γ.

Proposition 3.10: *Let $\Gamma \subseteq \mathbb{R}^d$ be a lattice and $S \in P(\Gamma)$. If $x \in \mathbb{R}^d$, then*

$$OC(Sx+\Gamma) = S[OC(x+\Gamma)]S^{-1}.$$

Proof: This is a consequence of Theorem 3.8 because $SRS^{-1} \in OC(\Gamma)$ if and only if $R \in OC(\Gamma)$, and $SRS^{-1}(Sx) - Sx \in \Gamma + SRS^{-1}\Gamma$ if and only if $Rx - x \in \Gamma + R\Gamma$. ■

Furthermore, one has the following inclusion property.

Proposition 3.11: *If Γ is a lattice in $\mathbb{R}^d$ and $x, y \in \mathbb{R}^d$, then for all $a, b \in \mathbb{Z}$,*

$$OC(x+\Gamma) \cap OC(y+\Gamma) \subseteq OC[(ax+by)+\Gamma].$$

Proof: Let $R \in OC(x+\Gamma) \cap OC(y+\Gamma)$. It follows from Theorem 3.8 that $R \in OC(\Gamma)$ and $Rax - ax, Rby - by \in \Gamma + R\Gamma$ for any $a, b \in \mathbb{Z}$. This implies that $R(ax+by) - (ax+by) \in \Gamma + R\Gamma$ and hence, $R \in OC[(ax+by)+\Gamma]$. ■

Corollary 3.12: *Let Γ be a lattice in $\mathbb{R}^d$ and $x = \frac{\ell}{n}$, where $\ell \in \Gamma$ and $n \in \mathbb{N}$. Then $OC(ax+\Gamma) = OC(x+\Gamma)$ for all $a \in \mathbb{Z}$ that are relatively prime to n.*

Proof: The inclusion $OC(x+\Gamma) \subseteq OC(ax+\Gamma)$ follows directly from Proposition 3.11. Since a and n are relatively prime, there exist integers b, c such that $ab + nc = 1$. Applying again Proposition 3.11 yields

$$OC(ax+\Gamma) \subseteq OC(abx+\Gamma) = OC[(ab+nc)\tfrac{\ell}{n} + \Gamma] = OC(x+\Gamma).$$

■

The next proposition compares the sets of coincidence isometries of shifts of similar lattices and is the analogue of Theorem 1.3 for shifted lattices.

Proposition 3.13: *Let Γ be a lattice in $\mathbb{R}^d$ and $x \in \mathbb{R}^d$.*

(i) *If $\lambda \in \mathbb{R}^+$ then $OC(\lambda x + \lambda\Gamma) = OC(x+\Gamma)$ with $\Sigma_{\lambda x+\lambda\Gamma}(R) = \Sigma_\Gamma(R)$ for all $R \in OC(\lambda x + \lambda\Gamma)$.*

(ii) *If $S \in O(d)$ then $OC(Sx + S\Gamma) = S[OC(x+\Gamma)]S^{-1}$ with $\Sigma_{Sx+S\Gamma}(R) = \Sigma_\Gamma(S^{-1}RS)$ for all $R \in OC(Sx+S\Gamma)$.*

Proof: Both statements follow from Theorem 3.8, Theorem 1.3 and Equation (3.4). One obtains that $R(\lambda x) - \lambda x \in \lambda\Gamma + R(\lambda\Gamma)$ if and only if $Rx - x \in \Gamma + R\Gamma$ and $(SRS^{-1})(Sx) - Sx \in S\Gamma + (SRS^{-1})S\Gamma$ if and only if $Rx - x \in \Gamma + R\Gamma$. ■

Note that Theorem 3.8 shows that $OC(x+\Gamma)$ is a subset of $OC(\Gamma)$. The set $OC(x+\Gamma)$ is certainly nonempty because the identity isometry $\mathbb{1}_d \in OC(x+\Gamma)$. It also follows from Theorem 3.8 that $OC(x+\Gamma)$ is closed under inverses, that is, $R^{-1} \in OC(x+\Gamma)$ whenever $R \in OC(x+\Gamma)$ because $R^{-1} \in OC(\Gamma)$ and $R^{-1}x - x \in \Gamma + R^{-1}\Gamma$. However, given R_1, $R_2 \in OC(x+\Gamma)$, the product $R_2 \cdot R_1$ is not necessarily in $OC(x+\Gamma)$. Thus, one obtains the following result.

Proposition 3.14: *For a given lattice $\Gamma \subseteq \mathbb{R}^d$ and $x \in \mathbb{R}^d$, $OC(x+\Gamma)$ is a group if and only if it is closed under composition, that is, for all R_1, $R_2 \in OC(x+\Gamma)$, the product $R_2 \cdot R_1 \in OC(x+\Gamma)$.*

As was the case for color coincidences of a coloring of Γ determined by some sublattice of Γ (refer to Proposition 2.13), the product of two coincidence isometries of $x+\Gamma$ whose coincidence indices are relatively prime is again a coincidence isometry of $x+\Gamma$. This is stated in the next proposition.

Proposition 3.15: *Let $\Gamma \subseteq \mathbb{R}^d$ be a lattice and $x \in \mathbb{R}^d$. If $R_1, R_2 \in OC(x+\Gamma)$ with $\Sigma(R_1)$ and $\Sigma(R_2)$ relatively prime, then $R_2R_1 \in OC(x+\Gamma)$.*

Proof: From Theorem 3.8, $R_j \in OC(\Gamma)$ and $R_jx - x \in \Gamma + R_j\Gamma$ for $j \in \{1,2\}$. The product $R_2R_1 \in OC(\Gamma)$ because $OC(\Gamma)$ is a group. In addition,

$$R_2R_1x - x = (\underbrace{R_2R_1x - R_2x}_{\in R_2(\Gamma+R_1\Gamma)}) + (\underbrace{R_2x - x}_{\in\Gamma+R_2\Gamma}) \in \Gamma + R_2\Gamma + R_2R_1\Gamma.$$

However, by Proposition 1.9, $R_2\Gamma = \Gamma(R_2) + R_2\Gamma(R_1)$ because $\Sigma(R_1)$ and $\Sigma(R_2)$ are relatively prime. Since $\Gamma(R_2) \subseteq \Gamma$ and $R_2\Gamma(R_1) \subseteq R_2R_1\Gamma$, $\Gamma + R_2\Gamma + R_2R_1\Gamma = \Gamma + R_2R_1\Gamma$ and so $R_2R_1 \in OC(x+\Gamma)$. ■

3.3. The sets $\mathcal{H}$, $AC(\Gamma)$, and $OC(x+\Gamma)$ as groupoids

Let Γ be a lattice in $\mathbb{R}^d$ and $x \in \mathbb{R}^d$, and consider a coloring of Γ induced by some sublattice Γ' of Γ. The sets $\mathcal{H}$, $AC(\Gamma)$, and $OC(x+\Gamma)$ share the following properties:

(i) They are subsets of some group G (for $\mathcal{H}$ and $OC(x+\Gamma)$, $G = OC(\Gamma)$, while $G = E(d)$ for $AC(\Gamma)$).
(ii) They contain the identity isometry $\mathbb{1}_d$.
(iii) They are closed under inverses.
(iv) They are not necessarily closed under composition.

These properties suggest that these sets might be algebraic structures more general than groups, such as groupoids. The following (algebraic) definition of a groupoid comes from [**66, 42**], and is equivalent to the one used in [**64**].

Definition 3.16: Let G be a set and $G^{(2)} \subseteq G \times G$, together with a product map $* : G^{(2)} \to G$, $(a,b) \mapsto a * b$, and inverse map ${}^{-1} : G \to G$. Then G is a *groupoid* if for all $a, b, c \in G$, the following axioms are satisfied:

A1. $(a^{-1})^{-1} = a$
A2. If $(a,b), (b,c) \in G^{(2)}$ then $(a*b, c), (a, b*c) \in G^{(2)}$ with $(a*b)*c = a*(b*c)$.
A3. $(a^{-1}, a), (a, a^{-1}) \in G^{(2)}$
A4. If $(a,b) \in G^{(2)}$ then $a^{-1} * (a * b) = b$ and $(a * b) * b^{-1} = a$.

The set $G^{(2)}$, referred to as the *set of composable pairs*, is the set of all ordered pairs in $G \times G$ for which the product $*$ is defined. Clearly, a group G is a groupoid (with $G^{(2)} = G \times G$). Conversely, a groupoid G with $G^{(2)} = G \times G$ must be a group.

Given a groupoid G and $a \in G$, the *domain* and *range* of a is defined as $d(a) := a^{-1} * a$ and $r(a) := a * a^{-1}$, respectively. The set $U_G := d(G) = r(G)$ is called the *unit space of* G. Elements of U_G are called *units* for the reason that $u * d(u) = u * (u^{-1} * u) = u$ and $r(u) * u = (u * u^{-1}) * u = u$ for all $u \in U_G$.

Lemma 3.17: *A groupoid G is a group if and only if $|U_G| = 1$.*

Proof: If G is a group then U_G consists of only the identity element of G. In the other direction, assume $U_G = \{u\}$ and take $(a,b) \in G \times G$. It follows from A3, A4, and A1 that $a*u = a*d(a) = (a^{-1})^{-1}*(a^{-1}*a) = a$ and $u*b = r(b)*b = (b*b^{-1})*(b^{-1})^{-1} = b$. Thus, $(a,u), (u,b) \in G^{(2)}$ and by A2, $(a*u, b) = (a,b) \in G^{(2)}$. Hence, $G^{(2)} = G \times G$ and G is a group. ∎

Now, if one views the sets $\mathcal{H}$, $AC(\Gamma)$, and $OC(x+\Gamma)$ as a groupoid, then the identity isometry $\mathbb{1}_d$ is the only unit of these sets. The following result is now immediate from Lemma 3.17.

Proposition 3.18: *Let $\Gamma \subseteq \mathbb{R}^d$ be a lattice and $x \in \mathbb{R}^d$, and consider a coloring of Γ determined by some sublattice of Γ. Then the sets $\mathcal{H}$, $AC(\Gamma)$, and $OC(x+\Gamma)$ are groupoids if and only if they are groups.*

3.4. Coincidences of a shifted square lattice

This entire section is devoted to the solution of the coincidence problem for a shifted square lattice. Some of the results here can be found in [**53**]. For the rest of the section, Γ is taken to be the square lattice viewed as the ring of Gaussian integers $\mathbb{Z}[i]$ (see Subsection 1.2.1), and $x \in \mathbb{C}$. In addition, as mentioned in Remark 1.11, $R_{z,\varepsilon} \in SOC(\Gamma)$ corresponds to multiplication by the complex number $\varepsilon\frac{z}{\overline{z}}$, while $T_{z,\varepsilon} = R_{z,\varepsilon} \cdot T_r \in OC(\Gamma) \setminus SOC(\Gamma)$, where T_r stands for complex conjugation.

The following lemma gives a criterion when $R_{z,\varepsilon} \in SOC(\Gamma)$ and $T_{z,\varepsilon} \in OC(\Gamma) \setminus SOC(\Gamma)$ are coincidence isometries of $x + \Gamma$.

Lemma 3.19: *Let $\Gamma = \mathbb{Z}[i]$, $x \in \mathbb{C}$, $R = R_{z,\varepsilon} \in SOC(\Gamma)$, and $T = R \cdot T_r$.*

(i) *$R \in SOC(x + \Gamma)$ if and only if $(\varepsilon z - \overline{z})x \in \Gamma$.*

(ii) *$T \in OC(x + \Gamma)$ if and only if $\varepsilon z\overline{x} - \overline{z}x \in \Gamma$.*

Proof: Since Γ is a principal ideal domain, ε is a unit in Γ, and z, $\overline{z}$ are relatively prime, one has

$$\Gamma + R\Gamma = \Gamma + \varepsilon\tfrac{z}{\overline{z}}\Gamma = \tfrac{1}{\overline{z}}\gcd(z, \overline{z})\Gamma = \tfrac{1}{\overline{z}}\Gamma.$$

By Theorem 3.8, $R \in SOC(x + \Gamma)$ if and only if $\varepsilon\frac{z}{\overline{z}}x - x \in \frac{1}{\overline{z}}\Gamma$, that is, whenever $(\varepsilon z - \overline{z})x \in \Gamma$.

Because T_r leaves Γ invariant, $\Gamma + T\Gamma = \frac{1}{\overline{z}}\Gamma$. Applying again Theorem 3.8 proves the corresponding result for T. ∎

3.4.1. The sets $SOC(x + \Gamma)$ and $OC(x + \Gamma)$. It turns out that the set of coincidence rotations of $x + \Gamma$ forms a group, as stated in the next theorem.

Theorem 3.20: *If $\Gamma = \mathbb{Z}[i]$ then $SOC(x+\Gamma)$ is a subgroup of $SOC(\Gamma)$ for all $x \in \mathbb{C}$.*

Proof: By Proposition 3.14, it is enough to show that $SOC(x + \Gamma)$ is closed under composition to prove the claim. Let $R_j = R_{z_j,\varepsilon_j} \in SOC(x + \Gamma)$ for $j \in \{1, 2\}$ and $g := \gcd(\overline{z_1}, z_2)$. Then $(\varepsilon_j z_j - \overline{z_j})x \in \Gamma$ from Lemma 3.19. Write $\overline{z_1} = \overline{h_1}g$ and $z_2 = h_2 g$, so that $\overline{h_1}$ and h_2 are relatively prime. Now,

$$\begin{aligned}\left(\varepsilon_2\varepsilon_1 h_2 h_1 - \overline{h_2 h_1}\right) x &= \tfrac{1}{g}\left(\varepsilon_2\varepsilon_1 z_2 h_1 - \overline{h_2 z_1}\right) x \\ &= \tfrac{1}{g}\big[\varepsilon_1 h_1 \underbrace{(\varepsilon_2 z_2 - \overline{z_2})x}_{\in\,\Gamma} + \overline{h_2} \underbrace{(\varepsilon_1 z_1 - \overline{z_1})x}_{\in\,\Gamma}\big] \in \tfrac{1}{g}\Gamma.\end{aligned}$$

Similarly, one obtains that $\left(\varepsilon_2\varepsilon_1 h_2 h_1 - \overline{h_2 h_1}\right) x \in \frac{1}{\overline{g}}\Gamma$. Together, they imply that

$$\left(\varepsilon_2\varepsilon_1 h_2 h_1 - \overline{h_2 h_1}\right) x \in \tfrac{1}{g}\Gamma \cap \tfrac{1}{\overline{g}}\Gamma = \tfrac{1}{g\overline{g}}\,\mathrm{lcm}\,(g, \overline{g})\Gamma = \Gamma.$$

This is because Γ is a principal ideal domain and g is relatively prime to $\overline{g}$. Hence, $R_2 \cdot R_1 = R_{h_2 h_1, \varepsilon_2\varepsilon_1} \in SOC(x + \Gamma)$ by Lemma 3.19. ∎

However, the situation is more complicated for $OC(x+\Gamma)$. One has the following results.

Lemma 3.21: *Let $\Gamma = \mathbb{Z}[i]$ and $x \in \mathbb{C}$. Then $OC(x + \Gamma)$ is a subgroup of $OC(\Gamma)$ if and only if for any coincidence reflections T_1, $T_2 \in OC(x + \Gamma)$, the coincidence rotation $T_2 \cdot T_1 \in SOC(x + \Gamma)$.*

Proof: It follows from Proposition 3.14 and Theorem 3.20 that it suffices to show that the product of a coincidence reflection and a coincidence rotation of $x + \Gamma$ is again a coincidence reflection of $x+\Gamma$. To this end, the same technique employed in the proof of Theorem 3.20 is used.

Let $R_j = R_{z_j,\varepsilon_j} \in SOC(\Gamma)$ for $j \in \{1,2\}$. Suppose R_2, $T_1 = R_1 \cdot T_r \in OC(x+\Gamma)$. Then $(\varepsilon_2 z_2 - \overline{z_2})x, \varepsilon_1 z_1 \overline{x} - \overline{z_1}x \in \Gamma$ from Lemma 3.19. Take $g := \gcd(\overline{z_1}, z_2)$, and express $\overline{z_1} = \overline{h_1}g$ and $z_2 = h_2 g$. One has

$$\begin{aligned}\varepsilon_2\varepsilon_1 h_2 h_1 \overline{x} - \overline{h_2 h_1}x &= \tfrac{1}{g}(\varepsilon_2\varepsilon_1 z_2 h_1 \overline{x} - \overline{h_2 z_1 x})\\ &= \tfrac{1}{g}\left[-\varepsilon_2\varepsilon_1 h_1\overline{(\varepsilon_2 z_2 - \overline{z_2})x} + \overline{h_2}(\varepsilon_1 z_1\overline{x} - \overline{z_1}x)\right] \in \tfrac{1}{g}\Gamma.\end{aligned}$$

In the same manner, one obtains $\varepsilon_2\varepsilon_1 h_2 h_1 \overline{x} - \overline{h_2 h_1}x \in \frac{1}{\overline{g}}\Gamma$. This means that

$$\varepsilon_2\varepsilon_1 h_2 h_1 \overline{x} - \overline{h_2 h_1}x \in \tfrac{1}{g}\,\Gamma \cap \tfrac{1}{\overline{g}}\,\Gamma = \Gamma.$$

Thus, $R_2 \cdot T_1 = R_{h_2 h_1, \varepsilon_2\varepsilon_1} \cdot T_r \in OC(x+\Gamma)$ by Lemma 3.19. Moreover, one has $T_1 \cdot R_2 = {R_2}^{-1} \cdot T_1 \in OC(x+\Gamma)$. ∎

Remark 3.22: Let $\Gamma = \mathbb{Z}[i]$, $x \in \mathbb{C}$, and $T_j = T_{z_j,\varepsilon_j} \in OC(x+\Gamma) \setminus SOC(x+\Gamma)$ for $j \in \{1,2\}$. Applying the same procedure used in the proofs of Theorem 3.20 and Lemma 3.21 to the product $T_2 \cdot T_1$ only leads to

$$\left(\varepsilon_2\overline{\varepsilon_1}h_2\overline{h_1} - \overline{h_2}h_1\right)x \in \tfrac{1}{g}\Gamma, \tag{3.5}$$

where $g := \gcd(z_1, z_2)$ and $z_j = h_j g$ for $j \in \{1,2\}$. It follows then from Lemma 3.19 that if z_1 were relatively prime to z_2, that is, if $g = 1$, then $T_2 \cdot T_1 = R_{h_2\overline{h_1}, \varepsilon_2\overline{\varepsilon_1}} \in SOC(x+\Gamma)$. This fact can also be deduced from Proposition 3.15, because if z_1 and z_2 were relatively prime, then so are $N(z_1) = \Sigma(R_1)$ and $N(z_2) = \Sigma(R_2)$. However, it is not always the case that the numerators z_1 and z_2 are relatively prime (an example of which will be given later). Thus, in general, $OC(x+\Gamma)$ is not a group.

Proposition 3.23: *Let $\Gamma = \mathbb{Z}[i]$ and $x \in \mathbb{C}$.*

(i) *If $OC(x+\Gamma)$ contains a reflection symmetry $T \in P(\Gamma)$ then $OC(x+\Gamma)$ is a subgroup of $OC(\Gamma)$. Moreover, $OC(x+\Gamma) = SOC(x+\Gamma) \rtimes \langle T\rangle$.*

(ii) *Suppose that $OC(x+\Gamma)$ does not contain any reflection symmetry $T \in P(\Gamma)$. Then the coincidence reflection $T_{z,\varepsilon} \notin OC(x+\Gamma)$ for all units ε of Γ whenever $R = R_{z,\varepsilon'} \in SOC(x+\Gamma)$ for some unit ε'.*

Proof:

(i) Because $T \in P(\Gamma)$, $T = T_{1,\varepsilon}$ for some unit ε of Γ. Thus, $\overline{x} \in \overline{\varepsilon}x + \Gamma$ by Lemma 3.19. Let $T_j = T_{z_j,\varepsilon_j} \in OC(x+\Gamma) \setminus SOC(x+\Gamma)$ for $j \in \{1,2\}$. If $g := \gcd(z_1, z_2)$ and $z_j = h_j g$ for $j \in \{1,2\}$, then it follows from Lemma 3.19 that

$$\begin{aligned} g\left(\varepsilon_2\overline{\varepsilon_1}h_2\overline{h_1} - \overline{h_2}h_1\right)\overline{x} &= \varepsilon_2\overline{\varepsilon_1}z_2\overline{h_1 x} - \overline{h_2}z_1\overline{x}\\ &= \overline{\varepsilon_1 h_1}(\varepsilon_2 z_2\overline{x} - \overline{z_2}x) - \overline{\varepsilon_1 h_2}(\varepsilon_1 z_1\overline{x} - \overline{z_1}x) \in \Gamma.\end{aligned}$$

Since $\overline{x} \in \overline{\varepsilon}x + \Gamma$, $\left(\varepsilon_2\overline{\varepsilon_1}h_2\overline{h_1} - \overline{h_2}h_1\right)x \in \frac{1}{\overline{g}}\Gamma$. This, together with (3.5), implies that $\left(\varepsilon_2\overline{\varepsilon_1}h_2\overline{h_1} - \overline{h_2}h_1\right)x \in \frac{1}{g}\,\Gamma \cap \frac{1}{\overline{g}}\,\Gamma = \Gamma$, and thus $T_2 \cdot T_1 \in OC(x+\Gamma)$. From Lemma 3.21, $OC(x+\Gamma)$ is a subgroup of $OC(\Gamma)$.

In addition, any coincidence reflection $T' = T_{z',\varepsilon'} \in OC(x+\Gamma)$ can be written as $T' = R' \cdot T$ where $R' = R_{z',\overline{\varepsilon}\varepsilon'} \in SOC(x+\Gamma)$. Hence, $OC(x+\Gamma)$ is the semidirect product of $SOC(x+\Gamma)$ and $\langle T \rangle$.

(ii) Assume otherwise, that is, $T_{z,\varepsilon} \in OC(x+\Gamma)$ for some unit ε of Γ. Since $R \in SOC(x+\Gamma)$, so is R^{-1}. Then $R^{-1} \cdot T_{z,\varepsilon} \in OC(x+\Gamma)$ by Lemma 3.21, which is a contradiction because $R^{-1} \cdot T_{z,\varepsilon} = T_{1,\overline{\varepsilon'}\varepsilon} \in P(\Gamma)$.

■

It can be surmised from Proposition 3.23 that when computing for $OC(x+\Gamma)$, it is advantageous to determine at the outset whether there is a reflection symmetry T that is in $OC(x+\Gamma)$. If such a T exists, then $OC(x+\Gamma)$ is a group and it is the semidirect product of $SOC(x+\Gamma)$ and $\langle T \rangle$. Otherwise, once $SOC(x+\Gamma)$ has already been identified, only those coincidence reflections $T_{z,\varepsilon} \in OC(\Gamma)$ for which $R_{z,\varepsilon'} \notin SOC(x+\Gamma)$ for all units ε' of Γ may be elements of $OC(x+\Gamma)$.

The following corollary describes exactly when a reflection symmetry is a coincidence isometry of $x+\Gamma$, and thus, gives an explicit version of Proposition 3.23(i).

Corollary 3.24: *Let $\Gamma = \mathbb{Z}[i]$ and $x \in \mathbb{C}$. Then $OC(x+\Gamma)$ is a subgroup of $OC(\Gamma)$ if one of the following conditions on x is satisfied:* $\mathrm{Re}\,(x) \in \frac{1}{2}\mathbb{Z}$, $\mathrm{Im}\,(x) \in \frac{1}{2}\mathbb{Z}$, *or* $\mathrm{Re}\,(x) \pm \mathrm{Im}\,(x) \in \mathbb{Z}$. *Furthermore, $OC(x+\Gamma) = SOC(x+\Gamma) \rtimes \langle T_{1,\varepsilon} \rangle$ where*

$$\varepsilon = \begin{cases} 1, & \text{if } \mathrm{Im}\,(x) \in \frac{1}{2}\mathbb{Z} \\ -1, & \text{if } \mathrm{Re}\,(x) \in \frac{1}{2}\mathbb{Z} \\ i, & \text{if } \mathrm{Re}\,(x) - \mathrm{Im}\,(x) \in \mathbb{Z} \\ -i, & \text{if } \mathrm{Re}\,(x) + \mathrm{Im}\,(x) \in \mathbb{Z}. \end{cases}$$

Proof: At least one of the given conditions on the components of x is satisfied if and only if $\varepsilon\overline{x} - x \in \Gamma$ for some unit ε of Γ. The latter implies that $T_{1,\varepsilon} \in OC(x+\Gamma)$ by Lemma 3.19. The claim now follows from Proposition 3.23(i) since $T_{1,\varepsilon} \in P(\Gamma)$. ■

3.4.2. Determination of $SOC(x+\Gamma)$ and $OC(x+\Gamma)$. We now turn to the actual computation of $OC(x+\Gamma)$ for specific values of x. Given $R_{z,\varepsilon} \in SOC(\Gamma)$, one sees from Lemma 3.19 the significance of the expression

$$\varepsilon z - \overline{z} = \begin{cases} 2i\,\mathrm{Im}\,(z)\,, & \text{if } \varepsilon = 1 \\ -2\mathrm{Re}\,(z)\,, & \text{if } \varepsilon = -1 \\ -[\mathrm{Re}\,(z) + \mathrm{Im}\,(z)](1-i), & \text{if } \varepsilon = i \\ -i[\mathrm{Re}\,(z) - \mathrm{Im}\,(z)](1-i), & \text{if } \varepsilon = -i\,. \end{cases} \tag{3.6}$$

Observe also that $\varepsilon z\overline{x} - \overline{z}x = \varepsilon\,(z\overline{x}) - \overline{(z\overline{x})}$. Hence, (3.6) can also be used to compute for $\varepsilon z\overline{x} - \overline{z}x$ for a given $T_{z,\varepsilon} \in OC(\Gamma) \setminus SOC(\Gamma)$.

Remark 3.25: Let $\Gamma = \mathbb{Z}[i]$. Then the following holds for all $R_{z,\varepsilon} \in SOC(\Gamma)$ and $T_{z,\varepsilon} \in OC(\Gamma) \setminus SOC(\Gamma)$ on account of the choice of z (see (1.2) and Remark 1.11):

(i) The rational integers $\mathrm{Re}\,(z)$ and $\mathrm{Im}\,(z)$ are relatively prime and are of different parity (that is, one is odd and the other is even).

(ii) $\mathrm{Re}\,(z) \neq 0$, and $z = 1$ whenever $\mathrm{Im}\,(z) = 0$.

The following theorem states the complete solution to the coincidence problem for $x+\Gamma$ when x has an irrational component.

Theorem 3.26: *Let $\Gamma=\mathbb{Z}[i]$ and $x=a+bi\in\mathbb{C}$, with $a,b\in\mathbb{R}$. If a or b is irrational then $OC(x+\Gamma)$ is a group of at most two elements. In particular, if*

(i) *a is irrational and b is rational then* $OC(x+\Gamma)=\begin{cases}\langle T_r\rangle, & \text{if } 2b\in\mathbb{Z}\\ \{\mathbb{1}\}, & \text{otherwise.}\end{cases}$

(ii) *a is rational and b is irrational then* $OC(x+\Gamma)=\begin{cases}\langle T_{1,-1}\rangle, & \text{if } 2a\in\mathbb{Z}\\ \{\mathbb{1}\}, & \text{otherwise.}\end{cases}$

(iii) *both a and b are irrational, and*

(a) *1, a, and b are rationally independent then $OC(x+\Gamma)=\{\mathbb{1}\}$.*

(b) *$a=\frac{p_1}{q_1}+\frac{p_2}{q_2}b$ where p_j, $q_j\in\mathbb{Z}$, and p_j is relatively prime to q_j for $j\in\{1,2\}$, with*

(i) *p_2q_2 even, then* $OC(x+\Gamma)=\begin{cases}\left\langle T_{p_2+q_2i,1}\right\rangle, & \text{if } q_1\mid 2q_2\\ \{\mathbb{1}\}, & \text{otherwise.}\end{cases}$

(ii) *p_2q_2 odd, then* $OC(x+\Gamma)=\begin{cases}\left\langle T_{\frac{p_2+q_2}{2}-\frac{p_2-q_2}{2}i,i}\right\rangle, & \text{if } q_1\mid q_2\\ \{\mathbb{1}\}, & \text{otherwise.}\end{cases}$

Proof: Suppose either a or b is irrational. If $R_{z,\varepsilon}\in SOC(x+\Gamma)$ then it follows from Lemma 3.19 that $\varepsilon z-\overline{z}=0$, else, $x=a+bi\in\mathbb{Q}(i)$. This means that $z=\varepsilon=1$ by (3.6) and Remark 3.25. Thus, $SOC(x+\Gamma)=\{\mathbb{1}\}$, where $\mathbb{1}$ is the identity isometry.

Assume $OC(x+\Gamma)$ includes two distinct reflections $T_j=T_{h_jg,\varepsilon_j}$ for $j\in\{1,2\}$, with h_1 and h_2 relatively prime. Since $\frac{1}{g}\Gamma\subseteq\mathbb{Q}(i)$ and $x\notin\mathbb{Q}(i)$, one obtains from (3.5) that $\varepsilon_2\overline{\varepsilon_1}h_2\overline{h_1}-\overline{h_2}h_1=0$. This implies that $\varepsilon_2\overline{\varepsilon_1}\,\frac{h_2\overline{h_1}}{\overline{h_2}h_1}=1$, and hence, $T_2\cdot T_1=\mathbb{1}$. Thus, $T_1={T_2}^{-1}=T_2$ and $OC(x+\Gamma)$ contains at most one reflection. That is, either $OC(x+\Gamma)=\{\mathbb{1}\}$ or $OC(x+\Gamma)=\{\mathbb{1},T_{z,\varepsilon}\}=\langle T_{z,\varepsilon}\rangle$ for some coincidence reflection $T_{z,\varepsilon}$.

Let $T_{z,\varepsilon}\in OC(\Gamma)\setminus SOC(\Gamma)$. One has

$$z\overline{x}=[a\mathrm{Re}\,(z)+b\mathrm{Im}\,(z)]+[a\mathrm{Im}\,(z)-b\mathrm{Re}\,(z)]i.$$

It follows from Remark 3.25 that if a is irrational and b is rational, then the real numbers $2\mathrm{Re}\,(z\overline{x})$, $\mathrm{Re}\,(z\overline{x})+\mathrm{Im}\,(z\overline{x})$, $\mathrm{Re}\,(z\overline{x})-\mathrm{Im}\,(z\overline{x})\notin\mathbb{Z}$. This means that $\varepsilon z\overline{x}-\overline{z}x\in\mathbb{Z}[i]$ if and only if $\varepsilon=1$ and $2\mathrm{Im}\,(z\overline{x})\in\mathbb{Z}$, that is, if $\varepsilon=z=1$ by (3.6) and Remark 3.25. If $z=1$, one has $2\mathrm{Im}\,(\overline{x})=-2b\in\mathbb{Z}$ and (i) now follows from Lemma 3.19. The proof of (ii) proceeds analogously.

Suppose now that both a and b are irrational and take $T_{z,\varepsilon}\in OC(\Gamma)$. From Lemma 3.19 and (3.6), one obtains that $T_{z,\varepsilon}\in OC(x+\Gamma)$ if and only if

$$a = \begin{cases} \frac{t}{2\mathrm{Im}(z)} + \frac{\mathrm{Re}(z)}{\mathrm{Im}(z)}b, & \text{if } \varepsilon = 1 \\ \frac{t}{2\mathrm{Re}(z)} - \frac{\mathrm{Im}(z)}{\mathrm{Re}(z)}b, & \text{if } \varepsilon = -1 \\ \frac{t}{\mathrm{Re}(z)+\mathrm{Im}(z)} + \frac{\mathrm{Re}(z)-\mathrm{Im}(z)}{\mathrm{Re}(z)+\mathrm{Im}(z)}b, & \text{if } \varepsilon = i \\ \frac{t}{\mathrm{Re}(z)-\mathrm{Im}(z)} - \frac{\mathrm{Re}(z)+\mathrm{Im}(z)}{\mathrm{Re}(z)-\mathrm{Im}(z)}b, & \text{if } \varepsilon = -i, \end{cases} \tag{3.7}$$

for some $t \in \mathbb{Z}$. Note that $\mathrm{Im}\,(z) \neq 0$, otherwise, b is rational. Also, $\mathrm{Re}\,(z) + \mathrm{Im}\,(z)$ and $\mathrm{Re}\,(z) - \mathrm{Im}\,(z)$ are both odd and relatively prime by Remark 3.25. In each case, one is able to write a as $a = c + d \cdot b$ where $c, d \in \mathbb{Q}$. This representation of a is unique, that is, if $a = e + f \cdot b$ where $e, f \in \mathbb{Q}$, then $c = e$ and $d = f$, because $b \notin \mathbb{Q}$.

Assume that $a = \frac{p_1}{q_1} + \frac{p_2}{q_2}b$ where p_j, $q_j \in \mathbb{Z}$ with p_j and q_j relatively prime for $j \in \{1, 2\}$. If p_2q_2 is even then a is expressible in the form (3.7) if and only if $\varepsilon = \pm 1$ and $q_1 \mid 2q_2$. In this instance, one can simply take $\varepsilon = 1$ and $z = p_2 + q_2 i$ so that $T_{z,\varepsilon} \in OC(x + \Gamma)$. On the other hand, if p_2q_2 is odd then a may be put in the form (3.7) if and only if $\varepsilon = \pm i$ and $q_1 \mid q_2$. This time, one may set $\varepsilon = i$ and $z = \frac{p_2+q_2}{2} - \frac{p_2-q_2}{2}i$, in order that $T_{z,\varepsilon} \in OC(x + \Gamma)$. This completes the proof. ∎

Example 3.27:

(i) Suppose $x = \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}}i$. One cannot write $\frac{1}{\sqrt{2}}$ as $c + d\frac{1}{\sqrt{3}}$, where $c, d \in \mathbb{Q}$, since $\sqrt{2} \notin \mathbb{Q}\left(\sqrt{3}\right)$. Hence, $OC(x + \Gamma) = \{\mathbb{1}\}$.

(ii) Let $x = \sqrt{2} - \frac{\sqrt{2}}{2}i$. Since $\sqrt{2} = \frac{0}{1} + \left(\frac{-2}{1}\right)\left(-\frac{\sqrt{2}}{2}\right)$ and $1 \mid (2 \cdot 1)$, one has $OC(x + \Gamma) = \langle T_{-2+i,1} \rangle$.

(iii) It is easy to verify that if $x = (e-2) + \frac{1}{7}(25 - 9e)i$ then $OC(x+\Gamma) = \langle T_{1+8i,i} \rangle$.

It only remains to consider the case when both components of x are rational. Suppose that $x = a + bi \in \mathbb{Q}(i)$ and write $x = \frac{p}{q}$, where p, $q \in \mathbb{Z}[i]$ with p and q relatively prime. The following lemma indicates that $SOC(x+\Gamma)$ ultimately depends on the denominator q of x.

Lemma 3.28: *Let $\Gamma = \mathbb{Z}[i]$, $x = \frac{p}{q}$ where p, $q \in \Gamma$ with p and q relatively prime, and $R = R_{z,\varepsilon} \in SOC(\Gamma)$. Then $R \in SOC(x + \Gamma)$ if and only if q divides $\varepsilon z - \overline{z}$. Consequently, $SOC(x + \Gamma) = SOC(\frac{1}{q} + \Gamma)$.*

Proof: By Lemma 3.19, $R \in SOC(x + \Gamma)$ if and only if $(\varepsilon z - \overline{z})x = \frac{(\varepsilon z - \overline{z})p}{q} \in \Gamma$. The latter is equivalent to $q \mid (\varepsilon z - \overline{z})$, because p and q are relatively prime. ∎

The following properties that relate $SOC(x + \Gamma)$ for different rational values of x are consequences of the divisibility condition set forth in Lemma 3.28.

Corollary 3.29: *If $q_1, q_2 \in \Gamma = \mathbb{Z}[i]$ such that $q_1 \mid q_2$, then*

$$SOC(\tfrac{1}{q_2} + \Gamma) \subseteq SOC(\tfrac{1}{q_1} + \Gamma).$$

Proof: If $R = R_{z,\varepsilon} \in SOC(\frac{1}{q_2} + \Gamma)$ then $q_2 \mid (\varepsilon z - \overline{z})$ by Lemma 3.28. Hence, q_1 also divides $\varepsilon z - \overline{z}$ and $R \in SOC(\frac{1}{q_1} + \Gamma)$. ∎

Corollary 3.30: *Suppose $q_1, q_2 \in \Gamma = \mathbb{Z}[i]$. Then*
$$SOC(\tfrac{1}{q_1} + \Gamma) \cap SOC(\tfrac{1}{q_2} + \Gamma) = SOC\big(\tfrac{1}{\mathrm{lcm}(q_1,q_2)} + \Gamma\big).$$
In particular, if q_1 and q_2 are relatively prime then
$$SOC(\tfrac{1}{q_1} + \Gamma) \cap SOC(\tfrac{1}{q_2} + \Gamma) = SOC\big(\tfrac{1}{q_1 q_2} + \Gamma\big).$$

Proof: The backward inclusion follows from Corollary 3.29 because q_1 and q_2 divide $\mathrm{lcm}(q_1, q_2)$. Suppose that $R = R_{z,\varepsilon} \in SOC(\frac{1}{q_1} + \Gamma) \cap SOC(\frac{1}{q_2} + \Gamma)$. It follows from Lemma 3.28 that $q_1 \mid (\varepsilon z - \overline{z})$ and $q_2 \mid (\varepsilon z - \overline{z})$. Since Γ is a principal ideal domain, $\mathrm{lcm}(q_1, q_2)$ also divides $\varepsilon z - \overline{z}$ and so $R \in SOC\big(\frac{1}{\mathrm{lcm}(q_1,q_2)} + \Gamma\big)$. Note that if q_1 is relatively prime to q_2, then $\mathrm{lcm}(q_1, q_2) = q_1 q_2$. ∎

One can generalize Corollary 3.30. That is, if the denominator q of x factorizes as $q = \prod\limits_j q_j^{r_k}$ where the q_j*'s* are primes in $\Gamma = \mathbb{Z}[i]$, then
$$SOC(\tfrac{1}{q} + \Gamma) = \bigcap_j SOC\left(\frac{1}{q_j^{r_k}} + \Gamma\right).$$

Corollary 3.31: *If $q \in \Gamma = \mathbb{Z}[i]$ then $SOC(\frac{1}{q}+\Gamma) = SOC(\frac{1}{\overline{q}}+\Gamma) = SOC\big(\frac{1}{\mathrm{lcm}\,(q,\overline{q})}+\Gamma\big)$.*

Proof: Since $\overline{\varepsilon z - \overline{z}} = -\overline{\varepsilon}(\varepsilon z - \overline{z})$ where $-\overline{\varepsilon}$ is a unit of $\mathbb{Z}[i]$, $q \mid (\varepsilon z - \overline{z})$ if and only if $\overline{q} \mid (\varepsilon z - \overline{z})$. The first equality then follows from Lemma 3.28. This now implies that $SOC(\frac{1}{q} + \Gamma) \cap SOC(\frac{1}{\overline{q}} + \Gamma) = SOC(\frac{1}{q} + \Gamma)$, and hence, the second equality is now a consequence of Corollary 3.30. ∎

The next proposition provides additional sufficient conditions when $OC(x + \Gamma)$ forms a group.

Proposition 3.32: *Let $x = \frac{p}{q}$ where $p, q \in \Gamma = \mathbb{Z}[i]$ with p and q relatively prime. If none of the prime factors of $N(q)$ is a splitting prime of Γ, then $OC(x + \Gamma)$ is a group.*

Proof: Again, it follows from Lemma 3.21 that it is sufficient to show that the product of any two coincidence reflections $T_1 = T_{z_1,\varepsilon_1}$ and $T_2 = T_{z_2,\varepsilon_2}$ of $x+\Gamma$ is in $SOC(x+\Gamma)$ to prove that $OC(x + \Gamma)$ forms a group.

Since none of the prime factors of $N(q)$ splits in Γ, the prime factorization of q consists only of powers of $(1 - i)$ and of inert primes of Γ. This means that $\overline{q} = \overline{u}q$ for some unit u of Γ. It follows from Lemma 3.19 that for $j \in \{1, 2\}$,
$$\varepsilon_j z_j \tfrac{\overline{p}}{\overline{q}} - \overline{z_j}\tfrac{p}{q} = \tfrac{u\varepsilon_j z_j \overline{p} - \overline{z_j} p}{q} \in \Gamma.$$
Hence, $q \mid (u\varepsilon_j z_j \overline{p} - \overline{z_j} p)$. Set $g := \gcd(z_1, z_2)$ and $z_j = h_j g$ for $j \in \{1, 2\}$. Then q divides $u\varepsilon_2 z_2 \overline{z_1 p} - u\varepsilon_1 \overline{z_2} z_1 \overline{p} = u\varepsilon_1 g\overline{gp}\left(\varepsilon_2\overline{\varepsilon_1} h_2 \overline{h_1} - \overline{h_2} h_1\right)$. However, u and ε_1 are units, and q is relatively prime to g, $\overline{g}$ and $\overline{p}$, and so $q \mid \left(\varepsilon_2\overline{\varepsilon_1} h_2 \overline{h_1} - \overline{h_2} h_1\right)$. Finally, because $T_2 \cdot T_1 = R_{h_2\overline{h_1}, \varepsilon_2\overline{\varepsilon_1}} \in SOC(\Gamma)$, the product $T_2 \cdot T_1 \in SOC(x + \Gamma)$ by Lemma 3.28. ∎

The next proposition renders useful results about coincidence rotations of $x + \Gamma$ and their corresponding coincidence indices whenever the denominator q of x is an odd rational integer.

Proposition 3.33: *Let $\Gamma = \mathbb{Z}[i]$ and $q \neq 1$ be an odd positive rational integer. If $R = R_{z,\varepsilon} \in SOC(\frac{1}{q} + \Gamma)$ then the following holds.*

(i) *For all units $\varepsilon' \neq \varepsilon$, $R_{z,\varepsilon'} \notin SOC(\frac{1}{q} + \Gamma)$.*
(ii) *The coincidence index $\Sigma(R)$ is not divisible by q.*
(iii) *If in addition q is prime and $q \equiv \pm 1 \pmod 8$, then $\Sigma(R)$ is a quadratic residue modulo q.*

Proof: By Lemma 3.28, $q \mid (\varepsilon z - \overline{z})$.

(i) Assume to the contrary that $R_{z,\varepsilon'} \in SOC(\frac{1}{q} + \Gamma)$ for some unit $\varepsilon' \neq \varepsilon$ of Γ. Then $q \mid (\varepsilon' z - \overline{z})$ from Lemma 3.28. This implies that q divides $(\varepsilon z - \overline{z}) - (\varepsilon' z - \overline{z}) = (\varepsilon - \varepsilon')z$. Since q is odd and $\varepsilon' \neq \varepsilon$, q and $\varepsilon - \varepsilon'$ are relatively prime. Thus, $q \mid z$ and because q is a rational integer, q divides both real and imaginary parts of z. This is impossible by the choice of z (see Remark 3.25(i)).
(ii) Assume otherwise, that is, q divides $\Sigma(R) = N(z) = z\overline{z}$. Since q divides $z(\varepsilon z - \overline{z}) = \varepsilon z^2 - z\overline{z}$, the rational integer q also divides z^2. This contradicts Remark 3.25(i).
(iii) If $\varepsilon = \pm 1$ then q divides exactly one of $\mathrm{Re}\,(z)$ and $\mathrm{Im}\,(z)$ by (3.6) and Remark 3.25(i). This means that $\Sigma(R) = [\mathrm{Re}\,(z)]^2 + [\mathrm{Im}\,(z)]^2$ is a quadratic residue modulo q. On the other hand, if $\varepsilon = \pm i$ then $\Sigma(R) \equiv 2[\mathrm{Im}\,(z)]^2 \not\equiv 0 \pmod q$ by (3.6) and Remark 3.25(i). The claim now follows, because 2 is a quadratic residue of a prime q if and only if $q \equiv \pm 1 \pmod 8$ [**43**, Theorem 95] and the product of two quadratic residues is still a quadratic residue [**43**, Theorem 85].

■

The ring of Gaussian integers $\Gamma = \mathbb{Z}[i]$ is a Euclidean domain. That is, for any $a, b \in \Gamma$ with $b \neq 0$, there exist $k, r \in \Gamma$ such that $a = kb + r$ and $N(r) \leq \frac{1}{2}N(b)$ [**43**, Theorem 216]. The next proposition makes use of this fact.

Proposition 3.34: *Let q be an odd rational integer and write $z = kq + r$ where $k, r \in \Gamma = \mathbb{Z}[i]$ and $N(r) < \frac{1}{2}N(q)$. Then there is a unique unit ε of Γ such that $R_{z,\varepsilon} \in SOC(\frac{1}{q} + \Gamma)$ if and only if $\overline{r} = \varepsilon r$, that is, r and $\overline{r}$ are associates in Γ.*

Proof: Note that $\varepsilon z - \overline{z} = \left(\varepsilon k - \overline{k}\right) q + (\varepsilon r - \overline{r})$.

Suppose $R_{z,\varepsilon} \in SOC(\frac{1}{q} + \Gamma)$ for some unit ε of Γ. Then by Lemma 3.28, $q \mid (\varepsilon z - \overline{z})$ and hence, $q \mid (\varepsilon r - \overline{r})$. Since q is odd, $(1-i)q$ still divides $\varepsilon r - \overline{r}$ (see (3.6)). Thus, $N((1-i)q) = 2N(q) \mid N(\varepsilon r - \overline{r})$. However, (3.6) implies that $N(\varepsilon r - \overline{r}) \leq 4N(r) < 2N(q)$. Therefore, $N(\varepsilon r - \overline{r}) = 0$ and so $\overline{r} = \varepsilon r$.

Conversely, suppose $\overline{r} = \varepsilon r$ for some unit ε of Γ. Then $\varepsilon r - \overline{r} = 0$ which implies that $q \mid (\varepsilon z - \overline{z})$. Hence, $R_{z,\varepsilon} \in SOC(\frac{1}{q} + \Gamma)$ by Lemma 3.28. The uniqueness of ε follows from Proposition 3.33(i). ■

Let $R = R_{z,\varepsilon} \in SOC(\Gamma)$ and q be an odd rational integer. Express z as $z = kq + r$, where $k, r \in \Gamma$ and $N(r) < \frac{1}{2}N(q)$. Observe that r and $\overline{r}$ are associates in Γ if and only if r is a (rational integer) multiple of 1, i, $1+i$, or $1-i$. If this is the case, then it follows from Proposition 3.34 that $R \in SOC(\frac{1}{q}+\Gamma)$ with

$$\varepsilon = \begin{cases} 1, & \text{if } r \in \mathbb{Z} \\ -1, & \text{if } r \in i\mathbb{Z} \\ i, & \text{if } r \in (1-i)\mathbb{Z} \\ -i, & \text{if } r \in (1+i)\mathbb{Z}. \end{cases}$$

Proposition 3.34 leads to the following lower bound on the coincidence index of a coincidence rotation of $\frac{1}{q}+\Gamma$, where q is an odd rational integer.

Corollary 3.35: *Let $\Gamma = \mathbb{Z}[i]$ and q be an odd rational integer. If $R = R_{z,\varepsilon} \in SOC(\frac{1}{q}+\Gamma) \setminus P(\Gamma)$ then $\Sigma(R) > \frac{1}{2}q^2$.*

Proof: Write $z = kq + r$ where $k, r \in \Gamma$ and $N(r) < \frac{1}{2}N(q)$. Suppose $\Sigma(R) = N(z) \leq \frac{1}{2}q^2 = \frac{1}{2}N(q)$. Then $k = 0$ and $r = z$. Since $\frac{z}{\bar{z}}$ is not a unit, $R \notin SOC(\frac{1}{q}+\Gamma)$ for all units ε of Γ by Proposition 3.34. ■

3.4.3. Some examples. We now explicitly compute $OC(x+\Gamma)$ for some values of $x \in \mathbb{Q}(i)$. It follows from Proposition 3.10 that it is enough to compute $OC(x+\Gamma)$ only for values of x in some fundamental domain of the symmetry group G of Γ (a crystallographic group of type $*442$). We choose this fundamental domain to be the triangular region $\left\{x \in \mathbb{C} : 0 \leq \mathrm{Im}\,(x) \leq \mathrm{Re}\,(x) \leq \frac{1}{2}\right\}$ (see Figure 8).

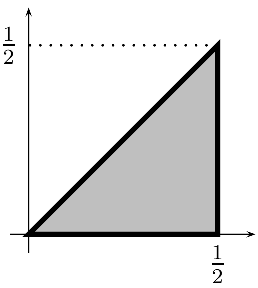


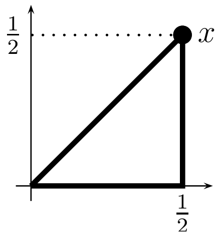
FIGURE 8. A fundamental domain of the symmetry group G of Γ

REMARK 3.36: Let $\Gamma = \mathbb{Z}[i]$ and $x \in \mathbb{C}$.

(i) For values of x in the fundamental domain of G in Figure 8, $OC(x+\Gamma)$ contains a reflection symmetry if and only if $\mathrm{Re}\,(x) = \frac{1}{2}$, $\mathrm{Im}\,(x) = 0$, or $\mathrm{Re}\,(x) = \mathrm{Im}\,(x)$ by Lemma 3.19. It follows then from Corollary 3.24 that $OC(x+\Gamma)$ is a subgroup of $OC(\Gamma)$ whenever x lies on the boundary of the fundamental domain.

(ii) The number of possible coincidence rotations and CSLs for a given index m of the shifted lattice $x+\Gamma$ shall be denoted by $\hat{f}_{x+\Gamma}(m)$ and $f_{x+\Gamma}(m)$, respectively.

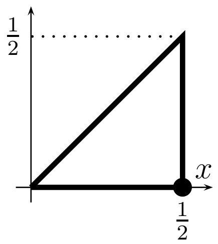
Example 3.37: $x = \frac{1}{2} + \frac{1}{2}i = \frac{1}{1-i}$



The denominator of x is $q = 1 - i$. One sees from (3.6) that $q \mid (\varepsilon z - \overline{z})$ for all numerators z and units ε of Γ. Lemma 3.28 and Corollary 3.24 imply that $SOC(x+\Gamma) = SOC(\Gamma)$ and $OC(x+\Gamma) = OC(\Gamma)$. Since $Sx - x \in \Gamma$ for all $S \in P(\Gamma)$, it follows from Proposition 3.9 that $\hat{f}_{x+\Gamma}(m) = \hat{f}_{\mathbb{Z}^2}(m)$ and $f_{x+\Gamma}(m) = f_{\mathbb{Z}^2}(m)$.

The results in Example 3.37 agree with those obtained in [**59**, Appendix A] (simply shift the center of a Delaunay cell into the origin, see also Remark 3.7). Observe that $(S)OC(x+\Gamma) = (S)OC(\Gamma)$ if and only if $x = \frac{m}{2} + \frac{n}{2}i$, where m and n are integers of the same parity.

Example 3.38: $x = \frac{1}{2}$

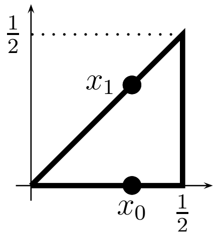


Here, x has denominator $q = 2$. Since the sum of $\mathrm{Re}\,(z)$ and $\mathrm{Im}\,(z)$ is odd by Remark 3.25(i), one obtains from (3.6) that for all numerators z, $q \mid (\varepsilon z - \overline{z})$ if and only if $\varepsilon = \pm 1$. Hence, by Lemma 3.28,

$$SOC(x+\Gamma) = \{R_{z,\varepsilon} \in SOC(\Gamma) : \varepsilon = \pm 1\} \cong C_2 \times \mathbb{Z}^{(\aleph_0)}.$$

By Corollary 3.24, $OC(x+\Gamma) = SOC(x+\Gamma) \rtimes \langle T_r \rangle$ and is a subgroup of $OC(\Gamma)$ of index 2. Note that $R_{1,-1} \in P(\Gamma)$ and $R_{1,-1}x - x = -1 \in \Gamma$. Hence, by Proposition 3.9, $f_{x+\Gamma}(m) = f_{\mathbb{Z}^2}(m)$ but $\hat{f}_{x+\Gamma}(m) = 2f_{x+\Gamma}(m) = \frac{1}{2}\hat{f}_{\mathbb{Z}^2}(m)$.

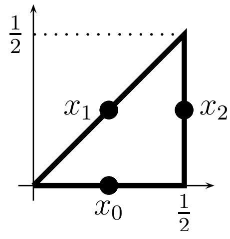
Example 3.39: $x_0 = \frac{1}{3}$ and $x_1 = \frac{1}{3} + \frac{1}{3}i$



Both x_0 and x_1 have denominator $q = 3$. Observe that if $r \in \Gamma$ lies inside the disk with center at 0 and radius $\sqrt{\frac{1}{2}N(q)} = \frac{3}{2}\sqrt{2}$, then r and $\overline{r}$ are associates in Γ. Hence, by Proposition 3.34, there is a unique unit ε of Γ for each numerator z so that

$R_{z,\varepsilon} \in SOC(\frac{1}{3}+\Gamma)$. Hence, $SOC(x_j+\Gamma) \cong \mathbb{Z}^{(\aleph_0)}$ for $j \in \{0,1\}$. In addition, by Corollary 3.24, $OC(x_j+\Gamma) = SOC(x_j+\Gamma) \rtimes \langle T_{1,i^j}\rangle$ and it is a subgroup of $OC(\Gamma)$ of index 4. Finally, $\hat{f}_{x_j+\Gamma}(m) = f_{x_j+\Gamma}(m) = f_{\mathbb{Z}^2}(m)$.

Example 3.40: $x_0 = \frac{1}{4}$, $x_1 = \frac{1}{4}+\frac{1}{4}i = \frac{1}{2(1-i)}$, and $x_2 = \frac{1}{2}+\frac{1}{4}i$

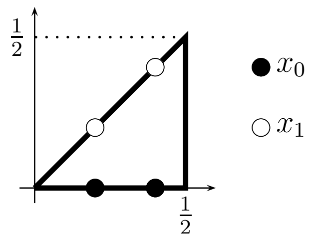


The denominator of x_0 and x_2 is $q=4$ while the denominator of x_1 is $q' = 2(1-i)$. Note that 2 divides both q and q' which means that $SOC(x_j+\Gamma) \subseteq SOC(\frac{1}{2}+\Gamma)$ for $j \in \{0,1,2\}$. Lemma 3.28, together with (3.6), yields

$$SOC(x_j+\Gamma) = \left\{R_{z,\varepsilon} \in SOC(\Gamma) : \varepsilon = (-1)^{\mathrm{Im}(z)}\right\} \cong \mathbb{Z}^{(\aleph_0)}.$$

It follows from Corollary 3.24 that $OC(x_j+\Gamma) = SOC(x_j+\Gamma) \rtimes \langle T_{1,i^j}\rangle$ and is a subgroup of index 4 in $OC(\Gamma)$. Moreover, $\hat{f}_{x_j+\Gamma}(m) = f_{x_j+\Gamma}(m) = f_{\mathbb{Z}^2}(m)$.

Example 3.41: $x_0 = \frac{1}{5}, \frac{2}{5}$ and $x_1 = \frac{1}{5}+\frac{1}{5}i, \frac{2}{5}+\frac{2}{5}i$



The denominator here is $q=5$. Write $z = 5k+r$ where $k, r \in \Gamma$ and $N(r) < \frac{25}{2}$. For all possible remainders r, r and $\overline{r}$ are not associates in Γ exactly when $N(r)=5$ or $N(r)=10$. The latter condition is equivalent to $5 \mid N(z)$, because $N(z) = 25N(k) + 10\mathrm{Re}\,(k\overline{r}) + N(r)$. Therefore, r and $\overline{r}$ are associates in Γ if and only if $5 \nmid N(z)$. It follows then from Proposition 3.34 that for all numerators z with $5 \nmid N(z)$, there is a unique unit ε of Γ such that $R_{z,\varepsilon} \in SOC(\frac{1}{5}+\Gamma)$. This means that $SOC(x_j+\Gamma) \cong \mathbb{Z}^{(\aleph_0)}$ for $j \in \{0,1\}$. Moreover, $OC(x_j+\Gamma)$ is a subgroup of $OC(\Gamma)$ with $OC(x_j+\Gamma) = SOC(x_j+\Gamma) \rtimes \langle T_{1,i^j}\rangle$ by Corollary 3.24. Furthermore,

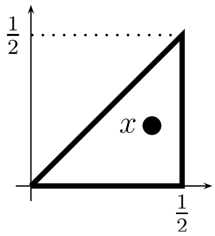
$$\hat{f}_{x_j+\Gamma}(m) = f_{x_j+\Gamma}(m) = \begin{cases} f_{\mathbb{Z}^2}(m), & \text{if } 5 \nmid m \\ 0, & \text{otherwise.} \end{cases}$$

The function $f_{x_j+\Gamma}(m)$ is still multiplicative and the Dirichlet series generating function for $f_{x_j}(m)$ is given by

$$\begin{aligned}\Phi_{x_j+\Gamma}(s) &= \sum_{m=1}^{\infty} \frac{f_{x_j+\Gamma}(m)}{m^s} = \prod_{\substack{p\equiv 1(4)\\ p\neq 5}} \frac{1+p^{-s}}{1-p^{-s}}\\ &= 1+\tfrac{2}{13^s}+\tfrac{2}{17^s}+\tfrac{2}{29^s}+\tfrac{2}{37^s}+\tfrac{2}{41^s}+\tfrac{2}{53^s}+\tfrac{2}{61^s}+\tfrac{2}{73^s}+\tfrac{2}{89^s}+\tfrac{2}{97^s}+\tfrac{2}{101^s}\\ &\quad+\tfrac{2}{109^s}+\tfrac{2}{113^s}+\tfrac{2}{137^s}+\tfrac{2}{149^s}+\tfrac{2}{157^s}+\tfrac{2}{169^s}+\tfrac{2}{173^s}+\tfrac{2}{181^s}+\tfrac{2}{193^s}+\tfrac{2}{197^s}\\ &\quad+\tfrac{4}{221^s}+\tfrac{2}{229^s}+\cdots.\end{aligned}$$

The next example gives an instance when the set of coincidence isometries of a shifted lattice does not form a group.

Example 3.42: $x = \frac{2}{5}+\frac{1}{5}i = \frac{i}{1+2i}$



The denominator of x is $q = 1+2i$. Since $5 = \operatorname{lcm}(q,\overline{q})$,

$$SOC(x+\Gamma) = SOC(\tfrac{1}{5}+\Gamma) \cong \mathbb{Z}^{(\aleph_0)}$$

by Corollary 3.31. Note that $OC(x+\Gamma)$ does not include a reflection symmetry since x lies in the interior of the fundamental domain of G in Figure 8 (see Remark 3.36(i)). Recall from Example 3.41 that there is a unique unit ε of Γ for each numerator z with $5 \nmid N(z)$ such that $R_{z,\varepsilon} \in SOC(\frac{1}{5}+\Gamma)$. This fact, together with Proposition 3.23(ii), implies that $5 \mid N(z)$ whenever $T_{z,\varepsilon} = R_{z,\varepsilon}\cdot T_r \in OC(x+\Gamma)$.

Given a numerator z with $5 \mid N(z)$, either $1+2i$ or $1-2i$ (and not both) appears in the factorization of z into primes of Γ. If $(1-2i) \mid z$ then $z\overline{x} \in \Gamma$ and $\varepsilon z\overline{x} - \overline{z}x = \varepsilon z\overline{x} - \overline{z\overline{x}} \in \Gamma$ for all units ε of Γ. On the other hand, if $(1+2i) \mid z$ then $\varepsilon z\overline{x} - \overline{z}x = \frac{i(-\varepsilon y - \overline{y})}{5}$, where $y = (1+2i)z$. Note that y is also a possible numerator corresponding to some coincidence rotation of Γ. This implies that $\varepsilon z\overline{x} - \overline{z}x \notin \Gamma$ for all units ε of Γ. Otherwise, 5 would divide $-\varepsilon y - \overline{y}$ and thus, by Lemma 3.28, $R_{y,-\varepsilon} \in SOC(\frac{1}{5}+\Gamma)$. This is impossible because $5 \mid N(y)$. Therefore, by Lemma 3.19,

$$OC(x+\Gamma) = SOC(x+\Gamma) \cup \{T_{z,\varepsilon} : (1-2i) \mid z\}.$$

We claim that $OC(x+\Gamma)$ is not a group. Indeed, let $T_j = T_{z,\varepsilon_j} \in OC(x+\Gamma)\setminus SOC(x+\Gamma)$ for $j \in \{1,2\}$ with $\varepsilon_1 \neq \varepsilon_2$. Then $T_2 \cdot T_1 = R_{1,\varepsilon_2\overline{\varepsilon_1}} \in P(\Gamma)$ with $\varepsilon_2\overline{\varepsilon_1} \neq 1$, which means that $T_2\cdot T_1 \notin SOC(x+\Gamma)$. It follows from Lemma 3.21 that $OC(x+\Gamma)$ is not a subgroup of $OC(\Gamma)$.

Since $SOC(x+\Gamma) = SOC(\frac{1}{5}+\Gamma)$, we conclude that $\hat{f}_{x+\Gamma}(m) = \hat{f}_{\frac{1}{5}+\Gamma}(m)$. Denote by $\hat{F}_{x+\Gamma}(m)$ the number of coincidence isometries of $x+\Gamma$ of index m. Note that

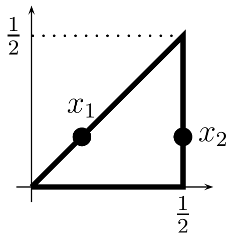
$Sx - x \notin \Gamma$ for each non-identity rotation $S \in P(\Gamma)$. Therefore, by Proposition 3.9, $f_{x+\Gamma}(m) = \hat{F}_{x+\Gamma}(m)$. Here, $f_{x+\Gamma}(m)$ is also multiplicative and is given by

$$f_{x+\Gamma}(p^r) = \begin{cases} 2, & \text{if } p \equiv 1 \pmod 4 \text{ and } p \neq 5 \\ 4, & \text{if } p = 5 \\ 0, & \text{otherwise,} \end{cases}$$

for primes p and $r \in \mathbb{N}$. The Dirichlet series generating function for $f_{x+\Gamma}(m)$ reads

$$\Phi_{x+\Gamma}(s) = \sum_{m=1}^{\infty} \frac{f_{x+\Gamma}(m)}{m^s} = \frac{1 + 3 \cdot 5^{-s}}{1 - 5^{-s}} \cdot \prod_{\substack{p \equiv 1(4) \\ p \neq 5}} \frac{1 + p^{-s}}{1 - p^{-s}}$$
$$= 1 + \tfrac{4}{5^s} + \tfrac{2}{13^s} + \tfrac{2}{17^s} + \tfrac{4}{25^s} + \tfrac{2}{29^s} + \tfrac{2}{37^s} + \tfrac{2}{41^s} + \tfrac{2}{53^s} + \tfrac{2}{61^s} + \tfrac{8}{65^s} + \tfrac{2}{73^s} + \ldots .$$

Example 3.43: $x_1 = \frac{1}{6} + \frac{1}{6}i = \frac{1}{3(1-i)}$ and $x_2 = \frac{1}{2} + \frac{1}{6}i = \frac{2-i}{3(1-i)}$

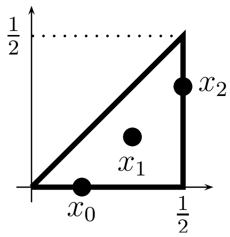


The denominator of both x_1 and x_2 is $q = 3(1-i)$. Since 3 and $1-i$ are relatively prime, one obtains from Corollary 3.30 and Examples 3.37 and 3.39 that

$$SOC(x_j + \Gamma) = SOC(\tfrac{1}{3} + \Gamma) \cap SOC(\tfrac{1}{1-i} + \Gamma) = SOC(\tfrac{1}{3} + \Gamma) \cong \mathbb{Z}^{(\aleph_0)},$$

for $j \in \{1, 2\}$. In addition, $OC(x_j + \Gamma) = SOC(x_j + \Gamma) \rtimes \langle T_{z,i^j} \rangle$ is a group by Corollary 3.24. Finally, $\hat{f}_{x_j+\Gamma}(m) = f_{x_j+\Gamma}(m) = f_{\mathbb{Z}^2}(m)$.

Example 3.44: $x_0 = \frac{1}{6}$, $x_1 = \frac{1}{3} + \frac{1}{6}i$, and $x_2 = \frac{1}{2} + \frac{1}{3}i$



The denominator of x_j is $q = 6 = 2 \cdot 3$ for $j \in \{0, 1, 2\}$. Hence, by Corollary 3.30,

$$SOC(x_j + \Gamma) = SOC(\tfrac{1}{2} + \Gamma) \cap SOC(\tfrac{1}{3} + \Gamma).$$

From Example 3.38, $SOC(\frac{1}{2} + \Gamma) = \{R_{z,\varepsilon} \in SOC(\Gamma) : \varepsilon = \pm 1\}$. Write $z = 3k + r$, where $k, r \in \Gamma$ and $N(r) < \frac{9}{2}$. Note that $N(z) = 9N(k) + 6\mathrm{Re}\,(k\overline{r}) + N(r) \equiv N(r) \pmod 3$. Also, for all possible remainders r, $\varepsilon = \frac{\overline{r}}{r} = \pm 1$ if and only if $N(r) \equiv 1 \pmod 3$. It follows from Proposition 3.34 that if z is a numerator with $N(z) \equiv 1 \pmod 3$, then $R_{z,\varepsilon} \in SOC(x_j + \Gamma)$ for some unique $\varepsilon \in \{1, -1\}$. Thus, $SOC(x_j + \Gamma) \cong \mathbb{Z}^{(\aleph_0)}$.

For $j \in \{0, 2\}$, $OC(x_j + \Gamma) = SOC(x_j + \Gamma) \rtimes \langle T_{1,i^j} \rangle$ is a group by Corollary 3.24. Also, $\hat{f}_{x_j+\Gamma}(m) = f_{x_j+\Gamma}(m)$ where

$$f_{x_j+\Gamma}(m) = \begin{cases} f_{\mathbb{Z}^2}(m), & \text{if } m \equiv 1 \pmod 3 \\ 0, & \text{otherwise.} \end{cases}$$

In this instance, $f_{x_j+\Gamma}(m)$ is not multiplicative. For example, $f_{x_j+\Gamma}(85) = 4$ but $f_{x_j+\Gamma}(5) \cdot f_{x_j+\Gamma}(17) = 0$.

Because x_1 lies in the interior of the fundamental domain of G in Figure 8, $OC(x_1 + \Gamma)$ does not contain a reflection symmetry (refer to Remark 3.36). It follows then from Proposition 3.23(ii) that if the coincidence reflection $T_{z,\varepsilon} \in OC(x_1 + \Gamma)$, then $N(z) \equiv 2 \pmod 3$. Conversely, suppose that z is a numerator with $N(z) \equiv 2 \pmod 3$. Note that the numerator of the shift x_1, $p = 2 + i$, is a factor of a splitting prime in Γ. Hence, $\pi := z\overline{p}$ is also a numerator corresponding to some coincidence rotation of Γ. In fact, because $N(\pi) = N(z) \cdot N(\overline{p}) \equiv 1 \pmod 3$, $R_{\pi,\varepsilon} \in SOC(\frac{1}{6} + \Gamma)$ for some unique $\varepsilon \in \{1, -1\}$. This means that 6 divides $\varepsilon\pi - \overline{\pi}$ by Lemma 3.28. One obtains then that $\varepsilon z\overline{x_1} - \overline{z}x_1 = \frac{1}{6}(\varepsilon\pi - \overline{\pi}) \in \Gamma$. Thus, $T_{z,\varepsilon} \in OC(x_1 + \Gamma)$ by Lemma 3.19. All in all, one has

$$OC(x_1 + \Gamma) = SOC(x_1 + \Gamma) \cup \left\{ T_{z,\varepsilon} \in OC(\Gamma) \setminus SOC(\Gamma) : N(z) \equiv 2 \pmod 3 \text{ and } \varepsilon = \begin{cases} 1, & \text{if } \operatorname{Im}(z\overline{p}) \equiv 0 \pmod 3 \\ -1, & \text{if } \operatorname{Re}(z\overline{p}) \equiv 0 \pmod 3 \end{cases} \right\}.$$

Since the factorization of $N(q) = 36$ consists only of powers of inert and ramified primes of Γ, $OC(x_1 + \Gamma)$ is again a group by Proposition 3.32 . Lastly, $\hat{f}_{x_1+\Gamma}(m) = \hat{f}_{\frac{1}{6}+\Gamma}(m)$ while $\hat{F}_{x_1+\Gamma}(m) = f_{x_1+\Gamma}(m) = f_{\mathbb{Z}^2}(m)$, where $\hat{F}_{x_1+\Gamma}(m)$ counts the number of coincidence isometries of $x_1 + \Gamma$ of a given index m.

3.5. Corresponding results for ℤ-modules

The concepts of *cosubmodule*, *index of a cosubmodule*, and *affine coincidence isometry* of $\mathbb{Z}$-modules in $\mathbb{R}^d$, as well as *cosubmodule*, (*linear*) *coincidence isometry*, *coincidence site module*, and *coincidence index of a coincidence isometry* of shifted $\mathbb{Z}$-modules are defined in exact analogy to Sections 3.1 and 3.2. In addition, by Remark 1.10, all results stated in both sections also hold for $\mathbb{Z}$-modules.

Moreover, general results obtained in Section 3.4 about the coincidences of a shifted square lattice are also true for planar n-modules with class number 1 (see Section 1.2.2). To be more exact, we write explicitly the corresponding results for planar n-modules $\mathcal{M}_n = \mathbb{Z}[\xi_n]$ without proof. Recall that coincidence rotations and coincidence reflections of $\mathcal{M}_n$ are also written as $R_{z,\varepsilon}$ and $T_{z,\varepsilon}$, respectively (refer to Remark 1.12).

Lemma 3.45: *Let $x \in \mathbb{C}$, $R = R_{z,\varepsilon} \in SOC(\mathcal{M}_n)$, and $T = R \cdot T_r$.*

(i) *$R \in SOC(x + \mathcal{M}_n)$ if and only if $(\varepsilon z - \overline{z})x \in \mathcal{M}_n$.*
(ii) *$T \in OC(x + \mathcal{M}_n)$ if and only if $\varepsilon z\overline{x} - \overline{z}x \in \mathcal{M}_n$.*

Theorem 3.46: *Let $x \in \mathbb{C}$.*

(i) *The set $SOC(x + \mathcal{M}_n)$ is a subgroup of $SOC(\mathcal{M}_n)$.*

(ii) *The set $OC(x + \mathcal{M}_n)$ is a subgroup of $OC(\mathcal{M}_n)$ if and only if for any coincidence reflections T_1, $T_2 \in OC(x + \mathcal{M}_n)$, the coincidence rotation $T_2 \cdot T_1 \in SOC(x + \mathcal{M}_n)$.*

(iii) *If $OC(x + \mathcal{M}_n)$ contains a reflection symmetry $T \in P(\mathcal{M}_n)$, then*
$$OC(x + \mathcal{M}_n) = SOC(x + \mathcal{M}_n) \rtimes \langle T \rangle$$
and is a subgroup of $OC(\mathcal{M}_n)$.

(iv) *If $OC(x+\mathcal{M}_n)$ does not contain any reflection symmetry $T \in P(\mathcal{M}_n)$, then the coincidence reflection $T_{z,\varepsilon} \notin OC(x+\mathcal{M}_n)$ for all units ε of $\mathcal{M}_n$ whenever $R_{z,\varepsilon'} \in SOC(x + \mathcal{M}_n)$ for some unit ε'.*

Theorem 3.47: *Let $x \in \mathbb{C}$.*

(i) *If $x \notin \mathbb{Q}(\xi_n)$ then $SOC(x + \mathcal{M}_n) = \{\mathbb{1}\}$.*

(ii) *Let $x = \frac{p}{q} \in \mathbb{Q}(\xi_n)$ where $p, q \in \mathcal{M}_n$ with p and q relatively prime, and $R = R_{z,\varepsilon} \in SOC(\mathcal{M}_n)$. Then $R \in SOC(x + \mathcal{M}_n)$ if and only if q divides $\varepsilon z - \overline{z}$. Consequently, $SOC(x + \mathcal{M}_n) = SOC(\frac{1}{q} + \mathcal{M}_n)$.*

Corollary 3.48:

(i) *If q_1, $q_2 \in \mathcal{M}_n$ such that $q_1 \mid q_2$, then $SOC(\frac{1}{q_2} + \mathcal{M}_n) \subseteq SOC(\frac{1}{q_1} + \mathcal{M}_n)$.*

(ii) *If q_1, $q_2 \in \mathcal{M}_n$ then*
$$SOC(\tfrac{1}{q_1} + \mathcal{M}_n) \cap SOC(\tfrac{1}{q_2} + \mathcal{M}_n) = SOC\big(\tfrac{1}{\operatorname{lcm}(q_1,q_2)} + \mathcal{M}_n\big).$$
In particular, if q_1 and q_2 are relatively prime then
$$SOC(\tfrac{1}{q_1} + \mathcal{M}_n) \cap SOC(\tfrac{1}{q_2} + \mathcal{M}_n) = SOC\big(\tfrac{1}{q_1 q_2} + \mathcal{M}_n\big),$$
and in general, if $q = \prod\limits_j q_j^{r_j}$ where the q_j's are primes in $\mathcal{M}_n$, then
$$SOC(\tfrac{1}{q} + \mathcal{M}_n) = \bigcap_j SOC\left(\frac{1}{q_j^{r_j}} + \mathcal{M}_n\right).$$

(iii) *If $q \in \mathcal{M}_n$ then $SOC(\frac{1}{q} + \mathcal{M}_n) = SOC(\frac{1}{\overline{q}} + \mathcal{M}_n) = SOC\big(\frac{1}{\operatorname{lcm}(q,\overline{q})} + \mathcal{M}_n\big)$.*

The proofs of these results proceed in the same fashion as the proofs of corresponding results in the square lattice case.

EXAMPLE 3.49: Consider the tenfold module $\mathcal{M} = \mathcal{M}_5 = \mathbb{Z}[\xi]$, where $\xi = \xi_5 = e^{2\pi i/5}$. Denote the golden ratio by $\tau = \frac{1}{2}\big(1+\sqrt{5}\,\big)$. For $z = a + b\xi + c\xi^2 + d\xi^3 \in \mathcal{M}$, one has

$$\varepsilon z - \overline{z} = \begin{cases} \xi^2(1-\xi)[(c-d)+b\tau], & \text{if } \varepsilon = 1 \\ (-2a+b)+(-b+c+d)\tau, & \text{if } \varepsilon = -1 \\ (1-\xi)[-a+(d-b)\tau], & \text{if } \varepsilon = \xi \\ \xi^3[(b+d-2c)+(a-b-d)\tau], & \text{if } \varepsilon = -\xi \\ \xi^3(1-\xi)[(b-c)+(a-d)\tau], & \text{if } \varepsilon = \xi^2 \\ \xi[(a+d)+(b+c-a-d)\tau], & \text{if } \varepsilon = -\xi^2 \\ \xi(1-\xi)[d+(c-a)\tau], & \text{if } \varepsilon = \xi^3 \\ \xi^4[(a-2b+c)+(-a-c+d)\tau], & \text{if } \varepsilon = -\xi^3 \\ \xi^4(1-\xi)[(a-b)-c\tau], & \text{if } \varepsilon = \xi^4 \\ \xi^2[(c-2d)+(a+b-c)\tau], & \text{if } \varepsilon = -\xi^4. \end{cases} \tag{3.8}$$

In particular, if $z = 1$,

$$\varepsilon z - \overline{z} = \begin{cases} 0, & \text{if } \varepsilon = 1 \\ -2, & \text{if } \varepsilon = -1 \\ -(1-\xi), & \text{if } \varepsilon = \xi \\ \xi^3\tau, & \text{if } \varepsilon = -\xi \\ \xi^3(1-\xi)\tau, & \text{if } \varepsilon = \xi^2 \\ \xi(1-\tau), & \text{if } \varepsilon = -\xi^2 \\ -\xi(1-\xi)\tau, & \text{if } \varepsilon = \xi^3 \\ \xi^4(1-\tau), & \text{if } \varepsilon = -\xi^3 \\ \xi^4(1-\xi), & \text{if } \varepsilon = \xi^4 \\ \xi^2\tau, & \text{if } \varepsilon = -\xi^4. \end{cases} \tag{3.9}$$

One sees from (3.9) that if $z = 1$, then $\varepsilon z - \overline{z}$ is a unit of $\mathcal{M}$ for $\varepsilon = -\xi^j$ for $1 \le j \le 4$. It follows from Lemma 3.45 that whenever $x \notin \mathcal{M}$, $SOC(x+\mathcal{M})$ must be a proper subgroup of $SOC(\mathcal{M})$.

Set $x = \frac{1}{2}(1 + i\cot\frac{\pi}{5}) = \frac{4+3\xi+2\xi^2+\xi^3}{5} = \frac{1}{1-\xi} \in \mathbb{Q}(\xi)$. The denominator of x is $q = 1-\xi$. We claim that for all numerators z, $q \mid (\varepsilon z - \overline{z})$ if and only if $\varepsilon = \xi^j$ for $0 \le j \le 4$. The reverse direction is clear from (3.8). Conversely, assume that $q \mid (\varepsilon z - \overline{z})$ for $\varepsilon = -\xi^j$ with $0 \le j \le 4$. Then by Lemma 3.45, $R_{z,\varepsilon} \in SOC(x+\mathcal{M})$. Take $R' = R_{\overline{z},1} \in SOC(x+\mathcal{M})$. Since $SOC(x+\mathcal{M})$ is a group, $R \cdot R' = R_{1,\varepsilon} \in SOC(x+\mathcal{M})$. A look at (3.9) shows that this is impossible and this completes the proof of our claim.

Hence, by Lemma 3.45,

$$SOC(x+\mathcal{M}) = \big\{R_{z,\varepsilon} \in SOC(\mathcal{M}) : \varepsilon = \xi^j, 0 \le j \le 4\big\} \cong C_5 \times \mathbb{Z}^{(\aleph_0)}$$

and is a subgroup of $SOC(\mathcal{M})$ of index 2. Furthermore, $-\overline{x} - x = -1 \in \mathcal{M}$. This means that the reflection symmetry $T_{1,-1} \in P(\mathcal{M})$ is a coincidence reflection of $x + \mathcal{M}$ by Lemma 3.45. It follows then from Theorem 3.46(iii) that $OC(x + \mathcal{M})$ forms a subgroup of $OC(\mathcal{M})$ of index 2 and is given by

$$OC(x + \mathcal{M}) = SOC(x + \mathcal{M}) \rtimes \langle T_{1,-1} \rangle.$$

CHAPTER 4

Coincidences of multilattices

The last chapter of this thesis deals with the solution of the coincidence problem for multilattices. By a multilattice, we mean the union of a lattice and a finite number of translated copies of the lattice. The first section considers the simplest case: the coincidences of a multilattice that includes only two distinct copies of a lattice. This leads to the solution of the coincidence problem for the diamond packing as well as for the 2×1–primitive rectangular lattice. The results are then extended to general multilattices in the following section. By treating a lattice as a multilattice consisting of some sublattice and all of its cosets, connections among color coincidences, the coincidence indices of the sublattice, and the coincidences of the cosets (viewed as shifted copies of the sublattice) are established. Examples involving primitive and centered rectangular lattices are given at the end of the chapter to illustrate all of these ideas.

4.1. The union of a lattice and a shifted copy of the lattice

Let Γ be a lattice in $\mathbb{R}^d$, and $x \in \mathbb{R}^d$ with $x \notin \Gamma$. Consider the union L of Γ and the shifted lattice $x + \Gamma$, that is, $L := \Gamma \cup (x + \Gamma)$. An $R \in O(d)$ is said to be a (*linear*) *coincidence isometry of* L if $L(R) := L \cap RL$ contains a cosublattice of Γ or $x + \Gamma$. The *coincidence index of* R *with respect to* L, denoted by $\Sigma_L(R)$, is the ratio of the density of points in L with the density of points in $L(R)$. Note that L is in general not a lattice and $\Sigma_L(R) < \infty$ is not necessarily an integer.

4.1.1. Solution of the coincidence problem for L. The following lemma characterizes the intersections $\Gamma \cap R(x + \Gamma)$ and $(x + \Gamma) \cap R\Gamma$. It is a special case of Lemma 4.13, which will be stated and proved in the next section.

Lemma 4.1: *Let* Γ *be a lattice in* $\mathbb{R}^d$*, and* $x \in \mathbb{R}^d \setminus \Gamma$*. Then*

(i) $\Gamma \cap R(x+\Gamma)$ *is a cosublattice of* Γ *if and only if* $R \in OC(\Gamma)$ *and* $Rx \in \Gamma + R\Gamma$*. In addition, if* $Rx \in \ell + R\Gamma$ *where* $\ell \in \Gamma$*, then* $\Gamma \cap R(x + \Gamma) = \ell + \Gamma(R)$ *with* $\ell \notin \Gamma(R)$*.*

(ii) $(x + \Gamma) \cap R\Gamma$ *is a cosublattice of* $x + \Gamma$ *if and only if* $R \in OC(\Gamma)$ *and* $x \in \Gamma + R\Gamma$*. In addition, if* $x \in \ell + R\Gamma$ *where* $\ell \in \Gamma$*, then* $(x + \Gamma) \cap R\Gamma = (x - \ell) + \Gamma(R)$*.*

With the help of Lemma 4.1, one can now describe the various instances when $R \in O(d)$ is a coincidence isometry of L, as well as the resulting intersection $L(R)$ and the coincidence index $\Sigma_L(R)$.

Theorem 4.2: *Let $L = \Gamma \cup (x + \Gamma)$, where Γ is a lattice in $\mathbb{R}^d$ and $x \in \mathbb{R}^d \setminus \Gamma$. Then $R \in O(d)$ is a coincidence isometry of L if and only if $R \in OC(\Gamma)$. Moreover, if $R \in OC(\Gamma)$ with*

(i) *x, Rx, and $Rx - x \notin \Gamma + R\Gamma$, then $L(R) = \Gamma(R)$ and $\Sigma_L(R) = 2\Sigma(R)$.*

(ii) *$Rx - x \in \ell + R\Gamma$ for some $\ell \in \Gamma$, and $x \notin \Gamma + R\Gamma$, then*
$$L(R) = \Gamma(R) \cup [(x + \ell) + \Gamma(R)]$$
and $\Sigma_L(R) = \Sigma(R)$.

(iii) *$Rx \in \ell + R\Gamma$ for some $\ell \in \Gamma$, and $x \notin \Gamma + R\Gamma$, then $L(R) = \Gamma(R) \cup [\ell + \Gamma(R)]$ with $\ell \notin \Gamma(R)$, and $\Sigma_L(R) = \Sigma(R)$.*

(iv) *$x \in \ell + R\Gamma$ for some $\ell \in \Gamma$, and $Rx \notin \Gamma + R\Gamma$, then*
$$L(R) = \Gamma(R) \cup [(x - \ell) + \Gamma(R)]$$
and $\Sigma_L(R) = \Sigma(R)$.

(v) *$x \in \ell_1 + R\Gamma$ and $Rx = \ell_2 + R\Gamma$ for some $\ell_1, \ell_2 \in \Gamma$, then*
$$L(R) = \Gamma(R) \cup [\ell_2 + \Gamma(R)] \cup [(x - \ell_1) + \Gamma(R)] \cup [(x + \ell_2 - \ell_1) + \Gamma(R)]$$
with $\ell_2 \notin \Gamma(R)$, and $\Sigma_L(R) = \frac{1}{2}\Sigma(R)$.

Proof: Write $L(R) = L \cap RL$ as
$$L(R) = (\Gamma \cap R\Gamma) \cup [\Gamma \cap R(x + \Gamma)] \cup [(x + \Gamma) \cap R\Gamma] \cup [(x + \Gamma) \cap R(x + \Gamma)].$$
The claim now follows directly from Theorem 3.8 and Lemma 4.1 ■

Thus, the set of coincidence isometries of L is precisely $OC(\Gamma)$. Furthermore, for any coincidence isometry R of L, the intersection $L(R)$ is the union of cosublattices of Γ and $x + \Gamma$, one of which is always the CSL $\Gamma(R)$.

4.1.2. Coincidences of the diamond packing. The *diamond packing* or *tetrahedral packing* is made up of two face-centered cubic (f.c.c.) lattices, wherein one of the f.c.c. lattice is a translate of the other by $\frac{1}{4}(a, a, a)$, with a being the length of the edges of a conventional unit cell of the f.c.c. lattice (see Figure 9). It is also known as the packing D_3^+ and is not a lattice [**17**]. An equivalent way of constructing the diamond packing as a motif of vertices of tetrahedrons and their barycenters can be found in [**73**]. The diamond packing occurs in nature as the crystal structure of certain materials such as diamond (hence, the name), tin, silicon, and germanium. Even though studies on grain boundaries of diamond appear in the literature [**46, 32, 57, 1**], no systematic study of the coincidences of the diamond packing has been done. Here, we use the results of the previous subsection to compute for the coincidence isometries, coincidence indices, and the resulting intersections of the diamond packing.

Take $\Gamma = \Gamma_F$ to be an f.c.c. lattice. We identify $\mathbb{R}^3$ with $\mathrm{Im}\,(\mathbb{H})$, and we associate Γ with $\Gamma = 2\mathrm{Im}\,(\mathbb{L}) \cup [(1, 1, 0) + 2\mathrm{Im}\,(\mathbb{L})] \cup [(0, 1, 1) + 2\mathrm{Im}\,(\mathbb{L})] \cup [(1, 0, 1) + 2\mathrm{Im}\,(\mathbb{L})]$ (see Subsection 1.2.3). The dual lattice of Γ is the body-centered cubic lattice $\Gamma^* = \Gamma_B = \mathrm{Im}\,(\mathbb{J})$, and the diamond packing is given by $D_3^+ = \Gamma \cup (x + \Gamma)$, where $x = \frac{1}{2}(1, 1, 1)$. Hence, the group of coincidence isometries of D_3^+ is $OC(\Gamma) = OC(\Gamma^*)$ by Theorems 4.2 and 1.4. Thus, a coincidence rotation $R = R_q$ of D_3^+ is parametrized by a primitive quaternion $q = (q_0, q_1, q_2, q_3)$ so that $R(x) = qxq^{-1}$ for all $x \in \mathrm{Im}\,(\mathbb{H})$ (see Subsection 1.2.4).

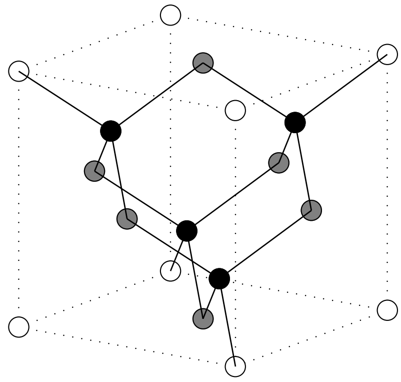


FIGURE 9. A unit cell of the diamond packing. The white and gray dots are part of the f.c.c. lattice while the black dots belong to the shifted f.c.c. lattice

Theorems 4.2 and 3.8 suggest that it is imperative that we compute for $OC(x+\Gamma)$ to determine the coincidence index of a coincidence isometry of D_3^+. To this end, note that $\Gamma + R\Gamma = (\Gamma^* \cap R\Gamma^*)^* = [\Gamma_B(R)]^*$, that is, $\Gamma + R\Gamma$ is the dual of the CSL $\Gamma_B(R)$. The next lemma, stated in [**81**] without proof, gives a spanning set for $\Gamma_B(R)$ over $\mathbb{Z}$.

Lemma 4.3: *Let $\Gamma_B = \mathrm{Im}\,(\mathbb{J})$ be the body-centered cubic lattice and $R = R_q \in SOC(\Gamma_B)$ where $q = (q_0, q_1, q_2, q_3)$ is a primitive quaternion. Denote by*

$$\begin{aligned} \mathbf{r_0} &:= \mathrm{Im}\,(q) = (q_1, q_2, q_3), & \mathbf{r_2} &:= \mathrm{Im}\,(q\mathbf{j}) = (-q_3, q_0, q_1), \\ \mathbf{r_1} &:= \mathrm{Im}\,(q\mathbf{i}) = (q_0, q_3, -q_2), & \mathbf{r_3} &:= \mathrm{Im}\,(q\mathbf{k}) = (q_2, -q_1, q_0). \end{aligned} \tag{4.1}$$

Then the CSL $\Gamma_B(R)$ is the $\mathbb{Z}$-span of the following vectors:

(i) $\mathbf{r_0}$, $\mathbf{r_1}$, $\mathbf{r_2}$, $\mathbf{r_3}$, $\frac{1}{2}(\mathbf{r_0}+\mathbf{r_1}+\mathbf{r_2}+\mathbf{r_3})$ *if* $|q|^2$ *is odd*

(ii) $\mathbf{r_0}$, $\frac{1}{2}(\mathbf{r_0}+\mathbf{r_1})$, $\frac{1}{2}(\mathbf{r_0}+\mathbf{r_2})$, $\frac{1}{2}(\mathbf{r_0}+\mathbf{r_3})$ *if* $|q|^2 \equiv 2 \pmod 4$

(iii) $\frac{1}{2}\mathbf{r_0}$, $\frac{1}{2}\mathbf{r_1}$, $\frac{1}{2}\mathbf{r_2}$, $\frac{1}{2}\mathbf{r_3}$ *if* $|q|^2 \equiv 0 \pmod 4$

Proof: Note that

$$R(\mathbf{r_0}) = \mathbf{r_0},\ R(q_0, -q_3, q_2) = \mathbf{r_1},\ R(q_3, q_0, -q_1) = \mathbf{r_2},\ \text{and } R(-q_2, q_1, q_0) = \mathbf{r_3}.$$

Hence, $\mathbf{r}_j \in \Gamma_B(R)$ for $0 \le j \le 3$. This means that for $0 \le j \le 3$, the lattice Γ_j generated by the vectors $\mathbf{r}_k$ with $k \ne j$ is a sublattice of Γ_B of index $2q_j|q|^2$, whenever $q_j \ne 0$ (see [**4**, proof of Proposition 3.2]). Beyond Γ_j, consider the lattice Γ' generated by all vectors $\mathbf{r}_j$, that is, $\Gamma' = \langle \mathbf{r_0}, \mathbf{r_1}, \mathbf{r_2}, \mathbf{r_3} \rangle_{\mathbb{Z}}$. Then Γ' contains each Γ_j as a sublattice, and is itself a sublattice of $\Gamma_B(R)$.

Now, observe that $q_0\mathbf{r_0} - q_1\mathbf{r_1} - q_2\mathbf{r_2} - q_3\mathbf{r_3} = 0$. This implies that each vector $\mathbf{r}_j$ may be written as a rational linear combination of $\mathbf{r}_k$, with $k \ne j$, as long as $q_j \ne 0$. Since q is primitive, $t\mathbf{r}_j$ with $t \in \mathbb{Z}$ is an integer linear combination of $\mathbf{r}_k$, $k \ne j$, if and only if $q_j \mid t$. Consequently, if $q_j \ne 0$, then Γ_j is of index q_j in Γ'. Thus, $[\Gamma_B(R) : \Gamma'] = \frac{2|q|^2}{\Sigma(R)}$.

If $|q|^2$ is odd then $\Sigma(R) = |q|^2$ (see Subsection 1.2.4), and so $[\Gamma_B(R) : \Gamma'] = 2$. Taking the vector $\frac{1}{2}(\mathbf{r_0}+\mathbf{r_1}+\mathbf{r_2}+\mathbf{r_3}) \in \Gamma_B(R) \setminus \Gamma'$ proves (i). On the other hand, $[\Gamma_B(R) : \Gamma'] = 4$ whenever $|q|^2 \equiv 2 \pmod 4$. Statement (ii) follows because $\frac{1}{2}(\mathbf{r_0} + \mathbf{r}_j) \in \Gamma_B(R) \setminus \Gamma'$ for $j \in \{1, 2, 3\}$. Finally, if $|q|^2 \equiv 0 \pmod 4$ then $[\Gamma_B(R) : \Gamma'] = 8$. In this instance, consider the lattice $\Gamma'' = \langle \frac{1}{2}\mathbf{r_0}, \frac{1}{2}\mathbf{r_1}, \frac{1}{2}\mathbf{r_2}, \frac{1}{2}\mathbf{r_3} \rangle_{\mathbb{Z}}$. Since $\Gamma' = 2\Gamma''$, Γ' is a sublattice of Γ'' of index 8. However, $\frac{1}{2}\mathbf{r}_j \in \Gamma_B(R)$ for $0 \le j \le 3$ because $|q|^2 \equiv 0 \pmod 4$. Hence, Γ'' is contained in $\Gamma_B(R)$, and thus, $\Gamma'' = \Gamma_B(R)$. This proves (iii). ∎

Remark 4.4: In the succeeding calculations, we embed $\mathrm{Im}\,(\mathbb{H})$ in $\mathbb{H}$ via the canonical projection. That is, vectors in $\mathrm{Im}\,(\mathbb{H})$ shall be treated as quaternions whose real part is 0.

We now proceed to determine $OC(x + \Gamma)$. First, observe that for $u \in \{\mathbf{e}, \mathbf{i}, \mathbf{j}, \mathbf{k}\}$, $R = R_q \in SOC(\Gamma)$, and $x \in \mathrm{Im}\,(\mathbb{H})$,

$$\langle Rx, \mathrm{Im}\,(qu) \rangle = \left\langle x, R^{-1}[\mathrm{Im}\,(qu)] \right\rangle = \left\langle x, q^{-1}[\mathrm{Im}\,(qu)]q \right\rangle = \langle x, uq \rangle . \tag{4.2}$$

Hence,

$$\langle Rx - x, \mathrm{Im}\,(qu) \rangle = \langle uq, x \rangle - \langle qu, x \rangle = \langle uq - qu, x \rangle .$$

Denote by $\times$ the usual vector (cross) product of two vectors in $\mathrm{Im}\,(\mathbb{H}) \cong \mathbb{R}^3$. Given $a, b, c \in \mathrm{Im}\,(\mathbb{H})$, one has $a \times b = \frac{1}{2}(ab - ba)$ and $\langle a \times b, c \rangle = \langle a, b \times c \rangle$ (see for instance, [**49**]). Since $uq - qu = u\mathrm{Im}\,(q) - \mathrm{Im}\,(q)\,u$ for $u \in \{\mathbf{i}, \mathbf{j}, \mathbf{k}\}$,

$$\langle Rx - x, \mathrm{Im}\,(qu) \rangle = -2 \langle \mathrm{Im}\,(q) \times u, x \rangle = -2 \langle \mathrm{Im}\,(q)\,, u \times x \rangle = -2 \langle q, u \times x \rangle .$$

Therefore, taking the vectors in (4.1) yields

$$\begin{aligned} &\langle Rx - x, \mathbf{r_0} \rangle = 0, &&\langle Rx - x, \mathbf{r_2} \rangle = -2 \langle q, \mathbf{j} \times x \rangle , \\ &\langle Rx - x, \mathbf{r_1} \rangle = -2 \langle q, \mathbf{i} \times x \rangle , &&\langle Rx - x, \mathbf{r_3} \rangle = -2 \langle q, \mathbf{k} \times x \rangle . \end{aligned} \tag{4.3}$$

Let $\ell \in \Gamma_B(R)$. Consider the following three possibilities:

`Case I:` $|q|^2$ is odd

By Lemma 4.3, $\ell = a\mathbf{r_0} + b\mathbf{r_1} + c\mathbf{r_2} + d\mathbf{r_3} + \frac{1}{2}e(\mathbf{r_0} + \mathbf{r_1} + \mathbf{r_2} + \mathbf{r_3})$, for some $a, b, c, d, e \in \mathbb{Z}$. It follows from (4.3) that

$$\langle Rx - x, \ell \rangle = -2 \langle q, (0, b, c, d) \times x \rangle - e \langle q, (0, 1, 1, 1) \times x \rangle .$$

Substituting $x = \frac{1}{2}(0, 1, 1, 1)$ gives

$$\langle Rx - x, \ell \rangle = - \langle q, (0, b, c, d) \times (0, 1, 1, 1) \rangle \in \mathbb{Z}$$

for all $a, b, c, d, e \in \mathbb{Z}$. This means that $Rx - x \in [\Gamma_B(R)]^* = \Gamma + R\Gamma$, and so $R_q \in SOC(x + \Gamma)$ whenever $|q|^2$ is odd by Theorem 3.8.

`Case II:` $|q|^2 \equiv 2 \pmod 4$

Write $\ell = a\mathbf{r_0} + \frac{1}{2}b(\mathbf{r_0} + \mathbf{r_1}) + \frac{1}{2}c(\mathbf{r_0} + \mathbf{r_2}) + \frac{1}{2}d(\mathbf{r_0} + \mathbf{r_3})$, for some $a, b, c, d \in \mathbb{Z}$. Thus,

$$\langle Rx - x, \ell \rangle = - \langle q, (0, b, c, d) \times x \rangle .$$

Set $x = \frac{1}{2}(0, 1, 1, 1)$. Since $|q|^2 \equiv 2 \pmod 4$, $q = r + 2s$ for some $s \in \mathbb{J}$ and $r \in \{(1, 1, 0, 0), (1, 0, 1, 0), (1, 0, 0, 1)\}$. Then

$$\langle Rx - x, \ell \rangle = -\tfrac{1}{2} \langle r, (0, b, c, d) \times (0, 1, 1, 1) \rangle - \underbrace{\langle s, (0, b, c, d) \times (0, 1, 1, 1) \rangle}_{\in \mathbb{Z}} \notin \mathbb{Z}$$

for some values of $b, c, d \in \mathbb{Z}$, because

$$\tfrac{1}{2}\langle r, (0,b,c,d) \times (0,1,1,1)\rangle = \begin{cases} \tfrac{1}{2}(c-d), & \text{if } r = (1,1,0,0) \\ \tfrac{1}{2}(d-b), & \text{if } r = (1,0,1,0) \\ \tfrac{1}{2}(b-c), & \text{if } r = (1,0,0,1). \end{cases}$$

Therefore, $Rx - x \notin \Gamma + R\Gamma$ and hence, $R_q \notin SOC(x+\Gamma)$ if $|q|^2 \equiv 2 \pmod 4$.

`Case III:` $|q|^2 \equiv 0 \pmod 4$

One can express ℓ as $\ell = \frac{1}{2}a\mathbf{r_0} + \frac{1}{2}b\mathbf{r_1} + \frac{1}{2}c\mathbf{r_2} + \frac{1}{3}d\mathbf{r_3}$ for some $a, b, c, d \in \mathbb{Z}$. This means that

$$\langle Rx - x, \ell\rangle = -\langle q, (0,b,c,d) \times x\rangle .$$

Take $x = \frac{1}{2}(0,1,1,1)$ and write $q = r + 2s$ where $s \in \mathbb{L}$ and $r = (1,1,1,1)$, which is possible because $|q|^2 \equiv 0 \pmod 4$. This yields

$$\langle Rx - x, \ell\rangle = -\langle s, (0,b,c,d) \times (0,1,1,1)\rangle \in \mathbb{Z},$$

for all $a, b, c, d \in \mathbb{Z}$. Consequently, $Rx - x \in \Gamma + R\Gamma$ and $R_q \in SOC(x+\Gamma)$ whenever $|q|^2 \equiv 0 \pmod 4$.

Therefore, $SOC(x+\Gamma) = \left\{R_q \in SOC(\Gamma) : |q|^2 \not\equiv 2 \pmod 4\right\}$.

It remains to identify those coincidence reflections $T = T_q \in OC(\Gamma)$ that are also in $OC(x+\Gamma)$ for $x = \frac{1}{2}(1,1,1)$. Since $T = -R$, where $R = R_q \in SOC(\Gamma)$, it follows from Theorem 3.8 that $T \in OC(x+\Gamma)$ if and only if $-Rx - x \in \Gamma + R\Gamma$.

By (4.2), one has $\langle -Rx - x, \mathrm{Im}\,(qu)\rangle = -\langle uq + qu, x\rangle$, for $u \in \{\mathbf{e}, \mathbf{i}, \mathbf{j}, \mathbf{k}\}$. Thus, the following holds (see (4.1)):

$$\begin{aligned} \langle -Rx - x, \mathbf{r_0}\rangle &= -2\langle q, x\rangle , & \langle Rx - x, \mathbf{r_2}\rangle &= -2[\mathrm{Re}\,(q)]\langle \mathbf{j}, x\rangle , \\ \langle -Rx - x, \mathbf{r_1}\rangle &= -2[\mathrm{Re}\,(q)]\langle \mathbf{i}, x\rangle , & \langle Rx - x, \mathbf{r_3}\rangle &= -2[\mathrm{Re}\,(q)]\langle \mathbf{k}, x\rangle . \end{aligned} \tag{4.4}$$

Consider an arbitrary element $\ell \in \Gamma_B(R)$. We take a look at the three different cases, as before. Note that Lemma 4.3 still holds for T, since T and R generate the same CSL.

`Case I:` $|q|^2$ is odd

If follows from (4.4) that

$$\begin{aligned} \langle -Rx - x, \ell\rangle = -2a\langle q, x\rangle &- 2[\mathrm{Re}\,(q)]\langle (0,b,c,d), x\rangle \\ &- e(\langle q, x\rangle + [\mathrm{Re}\,(q)]\langle (0,1,1,1), x\rangle) \end{aligned}$$

for some $a, b, c, d, e \in \mathbb{Z}$.

Set $x = \frac{1}{2}(0,1,1,1)$. Since $|q|^2 \equiv 1 \pmod 4$, one may write $q = r + 2s$ where $s \in \mathbb{J}$ and $r \in \{\mathbf{e}, \mathbf{i}, \mathbf{j}, \mathbf{k}\}$. Then

$$\begin{aligned} \langle -Rx - x, \ell\rangle = -a\langle q, (0,1,1,1)\rangle &- [\mathrm{Re}\,(q)](b+c+d) \\ &- e\underbrace{[3\mathrm{Re}\,(s) + \langle s, (0,1,1,1)\rangle]}_{\in\mathbb{Z}} - \tfrac{3}{2}e\mathrm{Re}\,(r) - \tfrac{1}{2}e\langle r, (0,1,1,1)\rangle \notin \mathbb{Z} \end{aligned}$$

for odd values of e. Therefore, $-Rx - x \notin \Gamma + R\Gamma$, and so $T_q \notin OC(x+\Gamma)$ whenever $|q|^2 \equiv 1 \pmod 4$.

`Case II:` $|q|^2 \equiv 2 \pmod 4$

Here,

$$\langle -Rx - x, \ell\rangle = -2a\,\langle q, x\rangle - (b+c+d)\,\langle q, x\rangle - [\mathrm{Re}\,(q)]\,\langle (0,b,c,d), x\rangle\,,$$

where $a, b, c, d \in \mathbb{Z}$.

Let x assume the value $\frac{1}{2}(0,1,1,1)$. Express q as $q = r + 2s$ for some $s \in \mathbb{J}$ and $r \in \{(1,1,0,0), (1,0,1,0), (1,0,0,1)\}$. Then

$$\langle -Rx - x, \ell\rangle = -a\,\langle q, (0,1,1,1)\rangle - (b+c+d)[1 + \underbrace{\mathrm{Re}\,(s) + \langle s, (0,1,1,1)\rangle}_{\in\mathbb{Z}}] \in \mathbb{Z}$$

for all $a, b, c, d \in \mathbb{Z}$. Hence, $-Rx - x \in \Gamma + R\Gamma$, which implies that $T_q \in OC(x+\Gamma)$ if $|q|^2 \equiv 2 \pmod 4$.

`Case III:` $|q|^2 \equiv 0 \pmod 4$

In this instance, one has

$$\langle -Rx - x, \ell\rangle = -a\,\langle q, x\rangle - [\mathrm{Re}\,(q)]\,\langle (0,b,c,d), x\rangle$$

for some $a, b, c, d \in \mathbb{Z}$.

Substitute $x = \frac{1}{2}(0,1,1,1)$ and write $q = r + 2s$, where $s \in \mathbb{L}$ and $r = (1,1,1,1)$. This yields

$$\langle -Rx - x, \ell\rangle = -a\,\langle s, (0,1,1,1)\rangle - (b+c+d)\mathrm{Re}\,(s) - \tfrac{1}{2}(3a+b+c+d) \notin \mathbb{Z}$$

whenever $3a + b + c + d$ is odd. Thus, $-Rx - x \notin \Gamma + R\Gamma$, and consequently, $T_q \notin OC(x+\Gamma)$ whenever $|q|^2 \equiv 0 \pmod 4$.

Hence, $OC(x+\Gamma) = SOC(x+\Gamma) \cup \big\{T_q \in OC(\Gamma) \setminus SOC(\Gamma) : |q|^2 \equiv 2 \pmod 4\big\}$.

We summarize the results for $OC(x+\Gamma)$ in the next lemma.

Lemma 4.5: *Let Γ be the f.c.c. lattice $\Gamma = 2\mathrm{Im}\,(\mathbb{L}) \cup [(1,1,0) + 2\mathrm{Im}\,(\mathbb{L})] \cup [(0,1,1) + 2\mathrm{Im}\,(\mathbb{L})] \cup [(1,0,1) + 2\mathrm{Im}\,(\mathbb{L})]$, and $x = \frac{1}{2}(1,1,1)$. Then $(S)OC(x+\Gamma)$ is a subgroup of $(S)OC(\Gamma)$ of index 2 given by*

$$SOC(x+\Gamma) = \big\{R_q \in SOC(\Gamma) : |q|^2 \not\equiv 2 \pmod 4\big\}\,,\ \text{and}$$
$$OC(x+\Gamma) = SOC(x+\Gamma) \cup \big\{T_q \in OC(\Gamma) \setminus SOC(\Gamma) : |q|^2 \equiv 2 \pmod 4\big\}\,.$$

If $f_{x+\Gamma}(m)$, $\hat{f}_{x+\Gamma}(m)$, and $\hat{F}_{x+\Gamma}(m)$ denote the number of CSLs, coincidence rotations, and coincidence isometries of $x+\Gamma$ of index m, respectively, then $f_{x+\Gamma}(m) = f_{\mathbb{Z}^3}(m)$, $\hat{f}_{x+\Gamma}(m) = 12 f_{x+\Gamma}(m)$, and $\hat{F}_{x+\Gamma}(m) = 24 f_{x+\Gamma}(m)$.

Proof: The explicit expressions for $(S)OC(x+\Gamma)$ were obtained from the computations preceding the lemma.

It follows from Theorem 1.13 that $R \in SOC(x+\Gamma)$ if and only if R is parametrized by a quaternion q with $|q|^2 = 2^t\alpha$, where t is an even integer and α is odd. Similarly, the coincidence reflection $T \in OC(x+\Gamma)$ if and only if T is parametrized by a quaternion q with $|q|^2 = 2^t\alpha$, where t and α are odd integers. With these two criteria, one concludes by going through all possible cases that $(S)OC(x+\Gamma)$ is closed under composition. Hence, by Proposition 3.14, $(S)OC(x+\Gamma)$ is a group.

Now, $Sx - x \in \Gamma$ for all $S \in P(\Gamma) \cap OC(x+\Gamma)$. Thus, by Proposition 3.9, $f_{x+\Gamma}(m) = f_{\mathbb{Z}^3}(m)$. Furthermore, expressions for $\hat{f}_{x+\Gamma}(m)$ and $\hat{F}_{x+\Gamma}(m)$ follow from the fact that there are 12 rotations $R_q \in P(\Gamma)$ with $|q|^2 \equiv 1 \pmod 4$ or $|q|^2 \equiv 0 \pmod 4$, and 12 rotoreflection symmetries $T_q \in P(\Gamma)$ with $|q|^2 \equiv 2 \pmod 4$. ∎

Finally, we show that both x and Rx are not in $\Gamma + R\Gamma$. To do this, it suffices to show that $\langle x, \ell\rangle \notin \mathbb{Z}$ and $\langle Rx, \ell\rangle \notin \mathbb{Z}$, respectively, for some $\ell \in \Gamma_B(R)$.

Given $a, b \in \mathbb{H}$, one has $\langle a, b\rangle = \frac{1}{2}\left(a\overline{b} + b\overline{a}\right)$ [**49**]. Thus, for $u \in \{\mathbf{e}, \mathbf{i}, \mathbf{j}, \mathbf{k}\}$, (with Remark 4.4 still in effect),

$$\langle x, \operatorname{Im}(qu)\rangle = \langle x, qu\rangle = \tfrac{1}{2}(x\overline{qu} + qu\overline{x}) = \langle x\overline{u}, q\rangle .$$

This means that (refer to (4.1))

$$\begin{aligned} \langle x, \mathbf{r_0}\rangle &= \langle x, q\rangle , & \langle x, \mathbf{r_2}\rangle &= -\langle x\mathbf{j}, q\rangle , \\ \langle x, \mathbf{r_1}\rangle &= -\langle x\mathbf{i}, q\rangle , & \langle x, \mathbf{r_3}\rangle &= -\langle x\mathbf{k}, q\rangle . \end{aligned} \tag{4.5}$$

Again, we look at the following three possibilities for an arbitrary $\ell \in \Gamma_B(R)$.

`Case I:` $|q|^2$ is odd

It follows from (4.5) that

$$\langle x, \ell\rangle = a\langle x, q\rangle - b\langle x\mathbf{i}, q\rangle - c\langle x\mathbf{j}, q\rangle - d\langle x\mathbf{k}, q\rangle + \tfrac{1}{2}e\langle x, q(1,1,1,1)\rangle ,$$

for some $a, b, c, d, e \in \mathbb{Z}$.

Take $x = \frac{1}{2}(0,1,1,1)$ and write $x = r + 2s$ for some $s \in \mathbb{J}$ and $r \in \{\mathbf{e}, \mathbf{i}, \mathbf{j}, \mathbf{k}\}$. Since

$$\tfrac{1}{2}e\langle x, q(1,1,1,1)\rangle = e[\tfrac{1}{4}\langle (0,1,1,1), r(1,1,1,1)\rangle + \langle (0,1,1,1), s'\rangle],$$

where $s' = \frac{1}{2}s(1,1,1,1) \in \mathbb{J}$, $\langle x, \ell\rangle \notin \mathbb{Z}$ if $a = b = c = d = 0$ and $e \not\equiv 0 \pmod 4$.

Therefore, $x \notin \Gamma + R\Gamma$. Also, since $Rx - x \in \Gamma + R\Gamma$ whenever $|q|^2$ is odd, $Rx \notin \Gamma + R\Gamma$.

`Case II:` $|q|^2 \equiv 2 \pmod 4$

Here,

$$\langle x, \ell\rangle = a\langle x, q\rangle + \tfrac{1}{2}b\langle x(1,-1,0,0), q\rangle + \tfrac{1}{2}c\langle x(1,0,-1,0), q\rangle + \tfrac{1}{2}d\langle x(1,0,0,-1), q\rangle$$

for some $a, b, c, d \in \mathbb{Z}$.

Substitute $x = \frac{1}{2}(0,1,1,1)$, and express $q = r + 2s$ where $s \in \mathbb{J}$ and $r \in \{(1,1,0,0), (1,0,1,0), (1,0,0,1)\}$. Several subcases arise.

(i) If $s \in \mathbb{L}$ then

$$a\langle x, q\rangle = \tfrac{1}{2}a + a\langle (0,1,1,1), s\rangle .$$

Hence, $\langle x, \ell\rangle \notin \mathbb{Z}$ if $b = c = d = 0$ and a is odd.

(ii) If $s \in \frac{1}{2}(1,1,1,1) + \mathbb{L}$ and $r \in \{(1,0,1,0), (1,0,0,1)\}$, then

$$\tfrac{1}{2}b\langle x(1,-1,0,0), q\rangle = b + \tfrac{1}{4}b\langle (1,1,0,2), r + 2t\rangle ,$$

for some $t \in \mathbb{L}$. Hence, $\langle x, \ell\rangle \notin \mathbb{Z}$ if $a = c = d = 0$ and $b \not\equiv 0 \pmod 4$.

(iii) If $s \in \frac{1}{2}(1,1,1,1) + \mathbb{L}$ and $r = (1,1,0,0)$, then

$$\tfrac{1}{2}c\langle x(1,0,-1,0), q\rangle = c + \tfrac{1}{4}c\langle (1,2,1,0), r + 2t\rangle ,$$

for some $t \in \mathbb{L}$. Hence, $\langle x, \ell\rangle \notin \mathbb{Z}$ if $a = b = d = 0$ and $c \not\equiv 0 \pmod 4$.

In all instances, $x \notin \Gamma + R\Gamma$. Also, $Rx \notin \Gamma + R\Gamma$ because $-Rx - x \in \Gamma + R\Gamma$ whenever $|q|^2 \equiv 2 \pmod 4$.

`Case III.` $|q|^2 \equiv 0 \pmod 4$

For this case, one obtains

$$\langle x, \ell \rangle = \tfrac{1}{2} a \langle x, q \rangle - \tfrac{1}{2} b \langle x\mathbf{i}, q \rangle - \tfrac{1}{2} c \langle x\mathbf{j}, q \rangle - \tfrac{1}{2} d \langle x\mathbf{k}, q \rangle$$

for some $a, b, c, d \in \mathbb{Z}$.

Set $x = \frac{1}{2}(0,1,1,1)$. Upon writing $q = r + 2s$ for some $s \in \mathbb{L}$ and $r = (1,1,1,1)$, one has

$$\tfrac{1}{2} a \langle x, q \rangle = \tfrac{1}{4} a [3 + 2 \langle (0,1,1,1), s \rangle].$$

Thus, $\langle x, \ell \rangle \notin \mathbb{Z}$ when $b = c = d = 0$ and $a \not\equiv 0 \pmod 4$. Hence, $x \notin \Gamma + R\Gamma$. Since $Rx - x \in \Gamma + R\Gamma$ if $|q|^2 \equiv 0 \pmod 4$, $Rx \notin \Gamma + R\Gamma$.

If $T = -R \in OC(\Gamma)$, then $\Gamma + T\Gamma = \Gamma + R\Gamma$ and $Tx \in \Gamma + T\Gamma$ if and only if $Rx \in \Gamma + R\Gamma$. This implies that x and Tx are also not in $\Gamma + T\Gamma$.

Applying Theorem 4.2, together with Lemma 4.5 and the preceding computations, yields the following solution of the coincidence problem for the diamond packing.

Theorem 4.6: *Let Γ be the f.c.c. lattice $\Gamma = 2\mathrm{Im}\,(\mathbb{L}) \cup [(1,1,0) + 2\mathrm{Im}\,(\mathbb{L})] \cup [(0,1,1) + 2\mathrm{Im}\,(\mathbb{L})] \cup [(1,0,1) + 2\mathrm{Im}\,(\mathbb{L})]$. Consider the diamond packing $D_3^+ = \Gamma \cup (x + \Gamma)$, where $x = \frac{1}{2}(1,1,1)$. Then the group of coincidence isometries of D_3^+ is $OC(\Gamma)$. In particular, $R = R_q \in SOC(\Gamma)$ is a coincidence rotation of D_3^+ with*

(i) *$D_3^+(R) = \Gamma(R)$ and $\Sigma_{D_3^+}(R) = 2\Sigma_\Gamma(R) = |q|^2$ if $|q|^2 \equiv 2 \pmod 4$.*

(ii) *$D_3^+(R) = \Gamma(R) \cup [(x + \ell) + \Gamma(R)]$, where $Rx - x \in \ell + R\Gamma$ with $\ell \in \Gamma$, and*

$$\Sigma_{D_3^+}(R) = \Sigma_\Gamma(R) = \begin{cases} |q|^2, & \text{if } |q|^2 \text{ is odd} \\ \frac{1}{4}|q|^2, & \text{if } |q|^2 \equiv 0 \pmod 4. \end{cases}$$

Also, $T = T_q \in OC(\Gamma) \setminus SOC(\Gamma)$ is a coincidence isometry of D_3^+ with

(i) *$D_3^+(T) = \Gamma(T)$ and* $\Sigma_{D_3^+}(T) = 2\Sigma_\Gamma(T) = \begin{cases} 2|q|^2, & \text{if } |q|^2 \text{ is odd} \\ \frac{1}{2}|q|^2, & \text{if } |q|^2 \equiv 0 \pmod 4. \end{cases}$

(ii) *$D_3^+(T) = \Gamma(T) \cup [(x + \ell) + \Gamma(T)]$, where $Tx - x \in \ell + T\Gamma$ with $\ell \in \Gamma$, and $\Sigma_{D_3^+}(T) = \Sigma_\Gamma(R) = \frac{1}{2}|q|^2$ if $|q|^2 \equiv 2 \pmod 4$.*

If $f_{D_3^+}(m)$ is the number of resulting intersections formed by coincidence isometries of D_3^+ of index m, then $f_{D_3^+}(m)$ is multiplicative and for primes p and $r \in \mathbb{N}$,

$$f_{D_3^+}(p^r) = \begin{cases} 1, & \text{if } p^r = 2 \\ 0, & \text{if } p = 2, r > 1 \\ (p+1)p^{r-1}, & \text{otherwise.} \end{cases}$$

The Dirichlet series generating function for $f_{D_3^+}(m)$ reads (see (1.4))

$$\Phi_{D_3^+}(s) = \sum_{m=1}^{\infty} \frac{f_{D_3^+}(m)}{m^s} = (1 + 2^{-s}) \cdot \Phi_{\mathbb{Z}^3}(s)$$
$$= 1 + \tfrac{1}{2^s} + \tfrac{4}{3^s} + \tfrac{6}{5^s} + \tfrac{4}{6^s} + \tfrac{8}{7^s} + \tfrac{12}{9^s} + \tfrac{6}{10^s} + \tfrac{12}{11^s} + \tfrac{14}{13^s} + \tfrac{8}{14^s} + \tfrac{24}{15^s} + \tfrac{18}{17^s} + \cdots .$$

REMARK 4.7: A related structure to the diamond packing is the *zincblende.* The crystal structure of some multi-element compounds like sphalerite, gallium arsenide, and cadmium telluride, take the form of the zincblende structure. The only difference between the zincblende structure and the diamond packing is that the former consists of two different types of atoms, one for each copy of the f.c.c. lattice, whereas in the latter all atoms are of the same type. In other words, one may view a zincblende structure as a coloring of the diamond packing where points belonging to the same f.c.c. lattice are assigned the same color.

Consider now the coincidence problem for the zincblende structure. Theorem 4.6 still gives the coincidences of the zincblende structure. The only difference is that coincidence isometries $R \in OC(\Gamma)$ for which $\Sigma_{D_3^+}(R) = \Sigma_\Gamma(R)$ involve a coincidence in both types of atoms, whereas for those with $\Sigma_{D_3^+}(R) = 2\Sigma_\Gamma(R)$, a coincidence occurs only for one type of atom (those located on Γ).

4.1.3. Application to lattice-sublattice relations. Suppose Γ_2 is a sublattice of index 2 in $\Gamma_1 \subseteq \mathbb{R}^d$. If $c_1 \in \Gamma_1 \setminus \Gamma_2$, then one may treat Γ_1 as the union of the lattice Γ_2 and the shifted copy $c_1 + \Gamma_2$ of Γ_2. This means that Theorem 4.2 is applicable in such a setting. Recall that $\mathcal{H}$ denotes the set of color coincidences of the coloring of Γ_1 determined by Γ_2 (see Section 2.2). Let $\mathcal{E} = \{R \in OC(\Gamma_1) : \Sigma_2(R) = \Sigma_1(R)\}$. The following corollary identifies the sets $\mathcal{E}$, $\mathcal{H}$, and $OC(c_1 + \Gamma_2)$.

Corollary 4.8: *Let Γ_1 be a lattice in $\mathbb{R}^d$, Γ_2 a sublattice of Γ_1 of index 2, $c_1 \in \Gamma_1 \setminus \Gamma_2$, and $R \in OC(\Gamma_1)$. Then*

(i) *$R \in \mathcal{E}$ if and only if exactly one of c_1, Rc_1, and $Rc_1 - c_1$ is in $\Gamma_2 + R\Gamma_2$.*
(ii) *$R \in \mathcal{H}$ if and only if both c_1 and Rc_1 are not in $\Gamma_2 + R\Gamma_2$.*
(iii) *$OC(c_1 + \Gamma_2) = (\mathcal{E} \cap \mathcal{H}) \cup [OC(\Gamma_2) \setminus (\mathcal{E} \cup \mathcal{H})]$. In particular, if $\mathcal{E} = \mathcal{H}$ then $OC(c_1 + \Gamma_2) = OC(\Gamma_2)$.*

Proof:

(i) This is a consequence of Theorem 4.2.
(ii) By Theorem 2.8 and Lemma 2.2, $R \in \mathcal{H}$ if and only if $\Gamma_2 \cap \Gamma_1(R) = R\Gamma_2 \cap \Gamma_1(R) = \Gamma_2(R)$. Theorem 4.2 shows that the latter is true exactly when c_1, $Rc_1 \notin \Gamma_2 + R\Gamma_2$.
(iii) By Theorem 3.8, $R \in OC(c_1 + \Gamma_2)$ if and only if $Rc_1 - c_1 \in \Gamma_2 + R\Gamma_2$. If the latter is true, then either both c_1 and Rc_1 are not in $\Gamma_2 + R\Gamma_2$, or both are elements of $\Gamma_2 + R\Gamma_2$. It now follows from Theorem 4.2, (i), and (ii) that the former is true if $R \in \mathcal{E} \cap \mathcal{H}$ while the latter occurs when $R \in OC(\Gamma_2) \setminus (\mathcal{E} \cup \mathcal{H})$. For the opposite inclusion, suppose $R \in (\mathcal{E} \cap \mathcal{H})$ or $R \in OC(\Gamma_2) \setminus (\mathcal{E} \cup \mathcal{H})$. In both instances, $Rc_1 - c_1 \in \Gamma_2 + R\Gamma_2$ by Theorem 4.2, (i), and (ii). Thus, $R \in OC(c_1 + \Gamma_2)$.

■

The Venn diagram in Figure 10, wherein the roman numerals represent the different cases in Theorem 4.2, shows the relationship among the sets $\mathcal{E}$, $\mathcal{H}$, and $OC(x + \Gamma_2)$ as described in Corollary 4.8. Note that $\mathcal{E} \cup \mathcal{H} \cup OC(c_1 + \Gamma_2) = OC(\Gamma_1)$.

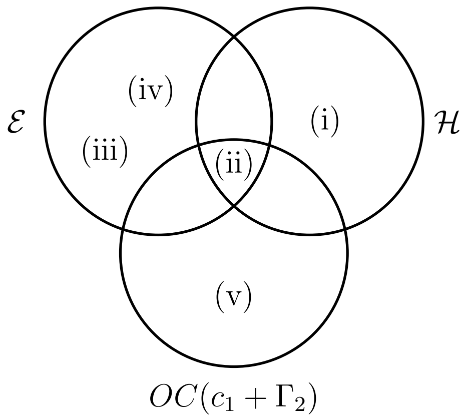


FIGURE 10. The sets $\mathcal{E}$, $\mathcal{H}$, and $OC(c_1 + \Gamma_2)$ for a sublattice Γ_2 of $\Gamma_1 = \Gamma_2 \cup (c_1 + \Gamma_2)$ of index 2. The numbers signify the corresponding cases in Theorem 4.2.

EXAMPLE 4.9: Let Γ_1 be a 2×1–primitive rectangular lattice. Identify Γ_1 with the $\mathbb{Z}$-span of $\frac{1}{2}$ and i in the complex plane, that is, $\Gamma_1 = \langle \frac{1}{2}, i \rangle_{\mathbb{Z}}$. Consider the square sublattice $\Gamma_2 = \mathbb{Z}[i]$ of index 2 in Γ_1. Thus, $\Gamma_1 = \Gamma_2 \cup (c_1 + \Gamma_2)$ with $c_1 = \frac{1}{2}$.

Recall from Example 3.38 that $SOC(c_1 + \Gamma_2) = \{R_{z,\varepsilon} \in SOC(\Gamma_2) : \varepsilon = \pm 1\}$ and $OC(c_1 + \Gamma_2) = SOC(c_1 + \Gamma_2) \rtimes \langle T_r \rangle$. Let $R = R_{z,\varepsilon} \in SOC(\Gamma_2)$. Then $c_1, Rc_1 \notin \Gamma_2 + R\Gamma_2 = \frac{1}{\overline{z}}\mathbb{Z}[i]$ because $2 \nmid \overline{z}$ and $2 \nmid \varepsilon z$ for all numerators z and units ε of Γ_2.

Therefore, by Theorem 4.2,

(i) $\Sigma_1(R) = 2\Sigma_2(R)$ and $\Gamma_1(R) = (z) = z\mathbb{Z}[i]$ if $R = R_{z,\varepsilon} \in SOC(\Gamma_2)$ with $\varepsilon = \pm i$.

(ii) $\Sigma_1(R) = \Sigma_2(R)$ and $\Gamma_1(R) = (z) \cup [c_1 + \ell + (z)]$, where $Rc_1 - c_1 \in \ell + R\Gamma_2$ with $\ell \in \Gamma_2$, if $R = R_{z,\varepsilon} \in SOC(\Gamma_2)$ with $\varepsilon = \pm 1$.

The same results hold for coincidence reflections $T = T_{z,\varepsilon}$ since $\Gamma_2 + T\Gamma_2 = \Gamma_2 + R\Gamma_2$ and $Tc_1 = Rc_1$. Hence, $\mathcal{H} = OC(\Gamma_2)$ and $\mathcal{E} = OC(c_1 + \Gamma_2)$ by Corollary 4.8.

Let $f_{\Gamma_1}(m)$ and $\hat{f}_{\Gamma_1}(m)$ be the number of CSLs and coincidence rotations of Γ_1 of index m, respectively. Then $\hat{f}_{\Gamma_1}(m) = 2f_{\Gamma_1}(m)$, and $f_{\Gamma_1}(m)$ is multiplicative given by

$$f_{\Gamma_1}(p^r) = \begin{cases} 1, & \text{if } p^r = 2 \\ 2, & \text{if } p \equiv 1 \pmod 4 \\ 0, & \text{otherwise,} \end{cases}$$

for primes p and $r \in \mathbb{N}$. The Dirichlet series generating function for $f_{\Gamma_1}(m)$ is then (see (1.3))

$$\begin{aligned} \Phi_{\Gamma_1}(s) = \sum_{m=1}^{\infty} \frac{f_{\Gamma_1}(m)}{m^s} &= (1 + 2^{-s}) \cdot \Phi_{\mathbb{Z}^2}(s) \\ &= 1 + \tfrac{1}{2^s} + \tfrac{2}{5^s} + \tfrac{2}{10^s} + \tfrac{2}{13^s} + \tfrac{2}{17^s} + \tfrac{2}{25^s} + \tfrac{2}{26^s} + \tfrac{2}{29^s} + \tfrac{2}{34^s} + \tfrac{2}{37^s} + \tfrac{2}{41^s} + \tfrac{2}{50^s} \\ &\quad + \tfrac{2}{53^s} + \tfrac{2}{58^s} + \tfrac{2}{61^s} + \tfrac{4}{65^s} + \tfrac{2}{73^s} + \cdots . \end{aligned}$$

EXAMPLE 4.10: This time, take Γ_1 to be the square lattice $\mathbb{Z}[i]$ and Γ_2 to be the 2×1–primitive rectangular sublattice $\langle 1, 2i\rangle_{\mathbb{Z}} = 2\langle \frac{1}{2}, i\rangle_{\mathbb{Z}}$ of Γ_1.

Recall from (1.3) that $\Sigma_1(R)$ is odd for all $R \in OC(\Gamma_1)$. It follows from Proposition 2.16 and Corollary 2.11 that $\mathcal{H} = \mathcal{E}$. Using the results from Example 4.9 and Theorem 1.3, one has $\mathcal{H} = \mathcal{E} = \{R_{z,\varepsilon} \in SOC(\Gamma_1) : \varepsilon = \pm 1\} \rtimes \langle T_r\rangle$. Observe that $\mathcal{H}$ is a group. Also, if $c_1 \in \Gamma_1 \setminus \Gamma_2$ then $OC(c_1+\Gamma_2) = OC(\Gamma_2) = OC(\Gamma_1)$ by Corollary 4.8.

The following example provides an alternative method of obtaining the result in Example 3.37.

EXAMPLE 4.11: Let $\Gamma_2 = \mathbb{Z}[i]$ and $c_1 = \frac{1}{2} + \frac{1}{2}i$. Note that $\Gamma_1 = \Gamma_2 \cup (c_1 + \Gamma_2)$ is again a square lattice. It follows then from Theorem 1.3 that $\mathcal{E} = OC(\Gamma_2)$. Since $[\Gamma_1 : \Gamma_2] = 2$ is relatively prime to $\Sigma_1(R)$ for all $R \in OC(\Gamma_2)$, $\mathcal{H} = \mathcal{E}$. Therefore, by Corollary 4.8, $OC(c_1 + \Gamma_2) = OC(\Gamma_2)$.

EXAMPLE 4.12: Let $\Gamma_1 = \mathbb{J}$ be the centered hypercubic lattice, and $\Gamma_2 = \mathbb{L}$ be the primitive hypercubic lattice that is a sublattice of Γ_1 of index 2. It has been shown in Example 2.22 that $\mathcal{E} = \mathcal{H}$ (see Proposition 2.23). Therefore, $OC(c_1 + \Gamma_2) = OC(\Gamma_2)$ for all $c_1 \in \Gamma_1 \setminus \Gamma_2$ by Corollary 4.8.

4.2. Multilattices

We now aim to generalize the results obtained in the previous section to finite unions of shifted copies of a lattice.

A subset L of $\mathbb{R}^d$ shall be called a *multilattice generated by the lattice* Γ *in* $\mathbb{R}^d$ if L is the union of Γ and a finite number of translated copies of Γ, that is, $L = \bigcup_{j=0}^{m-1} (x_j+\Gamma)$ where $x_j \in \mathbb{R}^d$, $m \in \mathbb{N}$, and $x_0 = 0$. An orthogonal transformation $R \in O(d)$ is a (*linear*) *coincidence isometry of* L if $L(R) := L \cap RL$ includes a cosublattice of some shifted lattice $x_j + \Gamma$, $0 \le j \le m-1$. The intersection $L(R)$ shall be referred to as a *coincidence site multilattice* (CSML) of L generated by R. The density of $L(R)$ in L, that is, the ratio of the density of points in L with the density of points in $L(R)$, is the *coincidence index of* R *with respect to* L, denoted by $\Sigma_L(R) < \infty$.

4.2.1. The coincidence problem for a multilattice.

The next lemma describes exactly when the intersection of a shifted lattice $x_k + \Gamma$ and the image of a shifted lattice $x_j + \Gamma$ under a linear isometry forms a cosublattice of $x_k + \Gamma$.

Lemma 4.13: *Suppose* Γ *is a lattice in* $\mathbb{R}^d$, $R \in O(d)$, *and* $x_j, x_k \in \mathbb{R}^d$. *Then* $(x_k + \Gamma) \cap R(x_j + \Gamma)$ *contains a cosublattice of* $x_k + \Gamma$ *if and only if* $R \in OC(\Gamma)$ *and* $Rx_j - x_k \in \Gamma + R\Gamma$. *Moreover, if* $Rx_j - x_k \in \ell_{j,k} + R\Gamma$ *with* $\ell_{j,k} \in \Gamma$, *then*

$$(x_k + \Gamma) \cap R(x_j + \Gamma) = (x_k + \ell_{j,k}) + \Gamma(R). \tag{4.6}$$

Proof: Write $(x_k+\Gamma) \cap R(x_j+\Gamma) = (x_k, \mathbb{1}_d)[\Gamma \cap (Rx_j - x_k, R)\Gamma]$. Then, the intersection $(x_k+\Gamma) \cap R(x_j+\Gamma)$ contains a cosublattice of $x_k + \Gamma$ if and only if $\Gamma \cap (Rx_j - x_k, R)\Gamma$ includes a cosublattice of Γ, that is, when $(Rx_j - x_k, R) \in AC(\Gamma)$. By Theorem 3.3, the latter is equivalent to saying that $R \in OC(\Gamma)$ and $Rx_j - x_k \in \Gamma + R\Gamma$. It follows from (3.1) that $(x_k + \Gamma) \cap R(x_j + \Gamma) = (x_k, \mathbb{1}_d)[\ell_{j,k} + \Gamma(R)] = (x_k + \ell_{j,k}) + \Gamma(R)$. ■

Lemma 4.1 now follows directly from Lemma 4.13 by taking $x_k = 0$, $x_j = x$, and vice versa. Theorem 3.8 is also a special case of Lemma 4.13 with $x_k = x_j = x$.

Equation (4.6) indicates that if $R \in OC(\Gamma)$ with $Rx_j - x_k \in \Gamma + R\Gamma$, then the intersection $(x_k + \Gamma) \cap R(x_j + \Gamma)$ does not only contain a cosublattice of $x_k + \Gamma$, but is itself a cosublattice of $x_k + \Gamma$. Furthermore, the index of the cosublattice $(x_k + \Gamma) \cap R(x_j + \Gamma)$ in $x_k + \Gamma$ is $\Sigma(R)$.

REMARK 4.14: Let $\Gamma \subseteq \mathbb{R}^d$ be a lattice, $R \in O(d)$, and $x_j, x_k \in \mathbb{R}^d$. It can be shown that $(x_k + \Gamma) \cap R(x_j + \Gamma)$ is a cosublattice of $x_k + \Gamma$ if and only if it is a cosublattice of $Rx_j + R\Gamma$. In fact, if $Rx_j - x_k \in Rt_{j,k} + \Gamma$ with $t_{j,k} \in \Gamma$ then

$$(x_k + \Gamma) \cap R(x_j + \Gamma) = (Rx_j - Rt_{j,k}) + \Gamma(R). \tag{4.7}$$

Since $\Sigma(R) = [\Gamma : \Gamma(R)] = [R\Gamma : \Gamma(R)]$, the cosublattice $(x_k + \Gamma) \cap R(x_j + \Gamma)$ is also of index $\Sigma(R)$ in $Rx_j + R\Gamma$.

The next result generalizes Theorem 4.2.

Theorem 4.15: *Let Γ be a lattice in $\mathbb{R}^d$ and $L = \bigcup_{j=0}^{m-1} (x_j + \Gamma)$ be a multilattice generated by Γ with $x_j \in \mathbb{R}^d$ for $0 \le j \le m-1$, $x_0 = 0$, and $x_j - x_k \notin \Gamma$ for $j \neq k$.*

(i) *Then the set of coincidence isometries of L is $OC(\Gamma)$.*

(ii) *Given an $R \in OC(\Gamma)$, define $\sigma := \{(x_j, x_k) : Rx_j - x_k \in \Gamma + R\Gamma\}$. Then $\Sigma_L(R) = \frac{m}{|\sigma|}\Sigma(R)$. In addition, if $Rx_j - x_k \in \ell_{j,k} + R\Gamma$ with $\ell_{j,k} \in \Gamma$, then*

$$L(R) = \bigcup_{(x_j, x_k) \in \sigma} [(x_k + \ell_{j,k}) + \Gamma(R)]. \tag{4.8}$$

Alternatively, if $Rx_j - x_k \in Rt_{j,k} + \Gamma$ with $t_{j,k} \in \Gamma$, then

$$L(R) = \bigcup_{(x_j, x_k) \in \sigma} [(Rx_j - Rt_{j,k}) + \Gamma(R)]. \tag{4.9}$$

Proof: For $j \neq k$, $(x_j + \Gamma) \cap (x_k + \Gamma) = \varnothing$ and $R(x_j + \Gamma) \cap R(x_k + \Gamma) = \varnothing$ since $x_j - x_k \notin \Gamma$. This implies that $L(R)$ may be written as the disjoint union

$$L(R) = L \cap RL = \bigcup_{j=0}^{m-1} \bigcup_{k=0}^{m-1} [(x_k + \Gamma) \cap R(x_j + \Gamma)]. \tag{4.10}$$

Suppose R is a coincidence isometry of L such that $L(R)$ includes a cosublattice of the shifted lattice $x_k + \Gamma$. This cosublattice must lie entirely in some intersection $(x_k + \Gamma) \cap R(x_j + \Gamma)$. Hence, $R \in OC(\Gamma)$ by Lemma 4.13. Conversely, if $R \in OC(\Gamma)$ then $L(R)$ contains the sublattice $\Gamma(R)$ of Γ. Thus, R is a coincidence isometry of L. This proves (i).

In (ii), $|\sigma| \neq 0$ because $(x_0, x_0) \in \sigma$. Note that $(x_k + \Gamma) \cap R(x_j + \Gamma) \neq \varnothing$ if and only if $(x_j, x_k) \in \sigma$. Then, applying (4.6) and (4.7) to each term in (4.10) yields (4.8) and (4.9), respectively. Now, each $(x_j, x_k) \in \sigma$ contributes a different shifted copy of $\Gamma(R)$ to $L(R)$. This means that $L(R)$ is made up of $|\sigma|$ distinct shifted copies of $\Gamma(R)$, each of which is of index $\Sigma(R)$ in the respective shifted copy of Γ or $R\Gamma$. Since L consists of m different shifted copies of Γ, the formula for $\Sigma_L(R)$ follows. ∎

Therefore, the set of coincidence isometries of the multilattice L generated by Γ is still $OC(\Gamma)$, albeit the coincidence indices of an $R \in OC(\Gamma)$ with respect to Γ and L are not necessarily equal. The CSML $L(R)$ is the union of cosublattices of shifted lattices in L, one of which must always be the CSL $\Gamma(R)$.

4.2.2. Lattices viewed as a multilattice generated by some sublattice. In general, a multilattice is not a lattice. However, a lattice Γ can always be treated as a multilattice generated by some sublattice of Γ, where the cosets of the sublattice of Γ play the role of shifted copies of the sublattice. Essentially, the situation here is the same as that in Section 2.1 (see also Figure 2). The difference, however, is that what are known in this setting are the coincidence indices and CSLs of the sublattice, and not those of the original lattice. From this perspective, we are able to see the connections among color coincidences of a coloring of Γ determined by some sublattice, the relation between the coincidence indices with respect to the lattice and the sublattice, and the coincidences of the cosets of the sublattice.

For the rest of this subsection, we take Γ_2 to be a sublattice of $\Gamma_1 \subseteq \mathbb{R}^d$ with $[\Gamma_1 : \Gamma_2] = m$. Write $\Gamma_1 = \bigcup_{j=0}^{m-1}(c_j + \Gamma_2)$, where $\{0 = c_0, c_1, \ldots, c_{m-1}\}$ is a complete set of coset representatives of Γ_2 in Γ_1. Given an $R \in OC(\Gamma_2)$, consider the sets

$$M := \{c_j + \Gamma_2 : Rc_j \in \Gamma_2 + R\Gamma_2\} \text{ and } N := \{c_k + \Gamma_2 : c_k \in \Gamma_2 + R\Gamma_2\}\,. \tag{4.11}$$

Both sets are clearly nonempty because $c_0 + \Gamma_2 = \Gamma_2 \in M, N$. The next lemma computes for the intersections $\Gamma_2 \cap \Gamma_1(R)$ and $R\Gamma_2 \cap \Gamma_1(R)$ using the sets M and N. Also, the sets J and K in (2.1) are formulated under this setting.

Lemma 4.16: *Suppose Γ_1 is a lattice in $\mathbb{R}^d$ having Γ_2 as a sublattice of index m, $\Gamma_2 = c_0 + \Gamma_2, c_1 + \Gamma_2, \ldots, c_{m-1} + \Gamma_2$ are the distinct cosets of Γ_2 in Γ_1, and $R \in OC(\Gamma_1) = OC(\Gamma_2)$.*

(i) *Given $c_j + \Gamma_2 \in M$ and $c_k + \Gamma_2 \in N$, let $Rc_j \in \ell_j + R\Gamma_2$ and $-c_k \in Rt_k + R\Gamma_2$ with $\ell_j, t_k \in \Gamma_2$. Then*

$$\begin{aligned} \Gamma_2 \cap \Gamma_1(R) &= \bigcup_{c_j+\Gamma_2 \in M} [\ell_j + \Gamma_2(R)] \text{ and} \\ R\Gamma_2 \cap \Gamma_1(R) &= \bigcup_{c_k+\Gamma_2 \in N} [-Rt_k + \Gamma_2(R)]. \end{aligned} \tag{4.12}$$

(ii) *The sets J and K in (2.1) are given by*

$$\begin{aligned} J &= \{c_j + \Gamma_2 : \exists\, c_k \text{ with } Rc_j - c_k \in \Gamma_2 + R\Gamma_2\} \text{ and} \\ K &= \{c_k + \Gamma_2 : \exists\, c_j \text{ with } Rc_j - c_k \in \Gamma_2 + R\Gamma_2\}\,. \end{aligned} \tag{4.13}$$

Proof: If $\sigma = \{(c_j, c_k) : Rc_j - c_k \in \Gamma_2 + R\Gamma_2\}$ then by (4.8) and (4.9),

$$\Gamma_1(R) = \bigcup_{(c_j,c_k)\in\sigma} [(c_k + \Gamma_2) \cap R(c_j + \Gamma_2)] = \begin{cases} \displaystyle\bigcup_{(c_j,c_k)\in\sigma} [(c_k + \ell_{j,k}) + \Gamma_2(R)] \\ \displaystyle\bigcup_{(c_j,c_k)\in\sigma} [(Rc_j - Rt_{j,k}) + \Gamma_2(R)] \end{cases} \tag{4.14}$$

where $Rc_j - c_k = \ell_{j,k} + Rt_{j,k}$ for some $\ell_{j,k}, t_{j,k} \in \Gamma_2$.

(i) Each coset $(c_k + \ell_{j,k}) + \Gamma_2(R)$ of $\Gamma_2(R)$ in $\Gamma_1(R)$ is contained in exactly one coset of Γ_2 in Γ_1. Thus, the union of the cosets of $\Gamma_2(R)$ in $\Gamma_1(R)$ with $c_k = c_0$ contains all elements of $\Gamma_1(R)$ in Γ_2. That is,

$$\Gamma_2 \cap \Gamma_1(R) = \bigcup_{(c_j, c_0) \in \sigma} [(c_0 + \ell_{j,0}) + \Gamma_2(R)] = \bigcup_{c_j + \Gamma_2 \in M} [\ell_j + \Gamma_2(R)].$$

Similarly, each coset $(Rc_j - Rt_{j,k}) + \Gamma_2(R)$ of $\Gamma_2(R)$ in $\Gamma_1(R)$ is a subset of the coset $Rc_j + R\Gamma_2$ of $R\Gamma_2$ in $R\Gamma_1$. Hence, the coset $(Rc_j - Rt_{j,k}) + \Gamma_2(R)$ lies in $R\Gamma_2$ whenever $c_j = c_0$, and

$$R\Gamma_2 \cap \Gamma_1(R) = \bigcup_{(c_0, c_k) \in \sigma} [(Rc_0 - Rt_{0,k}) + \Gamma_2(R)] = \bigcup_{c_k + \Gamma_2 \in N} [-Rt_k + \Gamma_2(R)].$$

(ii) One obtains from (4.14) that $(c_k + \Gamma_2) \cap \Gamma_1(R) \neq \varnothing$ if and only if $(c_j, c_k) \in \sigma$ for some c_j, $0 \leq j \leq m-1$. On the other hand, $(c_j + \Gamma_2) \cap \Gamma_1(R^{-1}) \neq \varnothing$, or equivalently, $R(c_j + \Gamma_2) \cap \Gamma_1(R) \neq \varnothing$ if and only if $(c_j, c_k) \in \sigma$ for some c_k, $0 \leq k \leq m-1$. The claim now follows from the definition of σ.

■

The following theorem interprets the values of s, t, u, and v defined in (2.5) in this situation. In addition, explicit expressions for $\Gamma_1(R)$ and $\Sigma_1(R)$ are specified.

Theorem 4.17: *Let Γ_2 be a sublattice of $\Gamma_1 \subseteq \mathbb{R}^d$, and $\{0 = c_0, c_1, \ldots, c_{m-1}\}$ be a complete set of coset representatives of Γ_2 in Γ_1.*

(i) *The following holds:*

$u := [\Gamma_2 \cap \Gamma_1(R) : \Gamma_2(R)] = |M|$

$v := [R\Gamma_2 \cap \Gamma_1(R) : \Gamma_2(R)] = |N|$

$s := [\Gamma_1(R) : R\Gamma_2 \cap \Gamma_1(R)] = |\{c_j + \Gamma_2 : \exists\, c_k \text{ with } Rc_j - c_k \in \Gamma_2 + R\Gamma_2\}|$

$t := [\Gamma_1(R) : \Gamma_2 \cap \Gamma_1(R)] = |\{c_k + \Gamma_2 : \exists\, c_j \text{ with } Rc_j - c_k \in \Gamma_2 + R\Gamma_2\}|$

(ii) *If $\sigma = \{(c_j, c_k) : Rc_j - c_k \in \Gamma_2 + R\Gamma_2\}$ then $\Sigma_1(R) = \frac{m}{|\sigma|}\Sigma_2(R)$, where $|\sigma| = t \cdot u = s \cdot v$ satisfying $s \mid m$, $t \mid m$, $u \mid s$, and $v \mid t$.*

(iii) *For each $c_k + \Gamma_2 \in K$, take $\tilde{\tilde{c}}_k = c_k + \ell_{j,k}$, where $Rc_j - c_k \in \ell_{j,k} + R\Gamma_2$ for some c_j, $0 \leq j \leq m-1$, with $\ell_{j,k} \in \Gamma_2$. Then*

$$\Gamma_1(R) = \bigcup_{c_k + \Gamma_2 \in K} \left(\tilde{\tilde{c}}_k + [\Gamma_2 \cap \Gamma_1(R)]\right).$$

Similarly, for each $c_j + \Gamma_2 \in J$, take $\tilde{c}_j = c_j - t_{j,k}$, where $Rc_j - c_k \in Rt_{j,k} + \Gamma_2$ for some c_k, $0 \leq k \leq m-1$, with $t_{j,k} \in \Gamma_2$. Then

$$\Gamma_1(R) = \bigcup_{c_j + \Gamma_2 \in J} (R\tilde{c}_j + [R\Gamma_2 \cap \Gamma_1(R)]).$$

Proof: The expressions for u and v in (i) follow directly from Lemma 4.16(i), while those of s and t are consequences of Theorem 2.4 and Lemma 4.16(ii).

The formula for $\Sigma_1(R)$ in (ii) is a restatement of Theorem 4.15(ii). This, together with (2.6), yields $|\sigma| = t \cdot u = s \cdot v$. The divisibility conditions are already known from Theorem 2.4.

By (4.14), $\tilde{\tilde{c}}_k \in (c_k + \Gamma_2) \cap \Gamma_1(R) \neq \varnothing$ for each $c_k + \Gamma_2 \in K$. It follows from Lemma 2.3 that

$$\Gamma_1(R) = \Gamma_1 \cap \Gamma_1(R) = \bigcup_{k=0}^{m-1} [(c_k + \Gamma_2) \cap \Gamma_1(R)] = \bigcup_{c_k+\Gamma_2 \in K} \left(\tilde{\tilde{c}}_k + [\Gamma_2 \cap \Gamma_1(R)]\right).$$

Similarly, for each $c_j + \Gamma_2 \in J$, $R\tilde{c}_j = Rc_j - Rt_{j,k} \in (Rc_j + R\Gamma_2) \cap \Gamma_1(R) \neq \varnothing$. Hence,

$$\Gamma_1(R) = R\Gamma_1 \cap \Gamma_1(R) = \bigcup_{j=0}^{m-1} [(Rc_j + R\Gamma_2) \cap \Gamma_1(R)] = \bigcup_{c_j+\Gamma_2 \in J} (R\tilde{c}_j + [R\Gamma_2 \cap \Gamma_1(R)])$$

by Lemma 2.3. This proves (iii). ■

Remark 4.18: Let Γ_2 be a sublattice of $\Gamma_1 \subseteq \mathbb{R}^d$ of index m. Write $\Gamma_1 = \bigcup_{j=0}^{m-1} (c_j + \Gamma_2)$ with $c_0 = 0$. For a fixed $R \in OC(\Gamma_1)$, consider the colorings of Γ_1, $\Gamma_1(R)$, and $\Gamma_1(R^{-1})$ determined by Γ_2 (see Section 2.1). Since $(c_k + \Gamma_2) \cap R(c_j + \Gamma_2) \cap \Gamma_1(R) \neq \varnothing$ if and only if $Rc_j - c_k \in \Gamma_2 + R\Gamma_2$, then the σ defined in (2.4) is exactly the same as the σ stated in Theorem 4.17(ii). Moreover, if D and E are the sets as defined in (2.8), and the sets M and N are those given in (4.11), then $D \cong M$ and $E \cong N$.

A close look at Theorem 4.17 reveals that it is not necessary to determine the set σ, that is, to check whether $Rc_j - c_k \in \Gamma_2 + R\Gamma_2$ is satisfied or not for every possible ordered pair (c_j, c_k) of coset representatives in order to reckon $|\sigma|$, and consequently $\Sigma_1(R)$. It is enough to compute for both u and t, or both v and s using Theorem 4.17(i). Furthermore, by choosing suitable coset representatives of Γ_2 in Γ_1 as specified in Theorem 4.17(iii), $\Gamma_1(R)$ can be expressed as the union of cosets of $\Gamma_2 \cap \Gamma_1(R)$ or $R\Gamma_2 \cap \Gamma_1(R)$ in $\Gamma_1(R)$.

Consider the coloring of Γ_1 determined by Γ_2. The next proposition describes the effect of a color coincidence of the coloring of Γ_1 on the colors in this setting.

Proposition 4.19: *Let $\Gamma_1 \subseteq \mathbb{R}^d$ be a lattice, Γ_2 be a sublattice of Γ_1 of index m, and $\{0 = c_0, c_1, \ldots, c_{m-1}\}$ be a complete set of coset representatives of Γ_2 in Γ_1. If R is a color coincidence of the coloring of Γ_1 determined by Γ_2, then R maps color c_j to c_k if and only if $Rc_j - c_k \in \Gamma_2 + R\Gamma_2$. In particular, R fixes color c_j if and only if $R \in OC(c_j + \Gamma_2)$.*

Proof: Let $c_j + \Gamma_2 \in J$. By (2.9), $R[(c_j + \Gamma_2) \cap \Gamma_1(R^{-1})] = (c_k + \Gamma_2) \cap \Gamma_1(R)$ for some $c_k + \Gamma_2 \in K$ whenever R sends color c_j to color c_k. This means that $(c_k + \Gamma_2) \cap R(c_j + \Gamma_2) \neq \varnothing$, and so $Rc_j - c_k \in \Gamma_2 + R\Gamma_2$.

In the other direction, suppose that $(c_j, c_k) \in \sigma = \{(c_j, c_k) : Rc_j - c_k \in \Gamma_2 + R\Gamma_2\}$. Since R is a color coincidence, σ must be a permutation. It follows then from (4.14) that

$$R[(c_j+\Gamma_2)\cap\Gamma_1(R^{-1})] = R(c_j+\Gamma_2)\cap\Gamma_1(R) = (c_k+\Gamma_2)\cap R(c_j+\Gamma_2) = (c_k+\Gamma_2)\cap\Gamma_1(R).$$

Hence, R maps the color c_j to c_k. The particular case follows from Theorem 3.8. ■

Recall that $\mathcal{H}$ denotes the set of color coincidences of the coloring of Γ_1 determined by Γ_2, while the set $\mathcal{E}$ consists of all $R \in OC(\Gamma_1) = OC(\Gamma_2)$ for which $\Sigma_1(R) = \Sigma_2(R)$. Given a coset $c_j + \Gamma_2$ of Γ_2 in Γ_1, the subgroup (of the factor group Γ_1/Γ_2) that it generates shall be written as $\langle c_j + \Gamma_2 \rangle$. The next proposition characterizes the sets $\mathcal{H}$ and $\mathcal{E}$. It also specifies how the various sets $OC(c_j + \Gamma_2)$ are related.

Proposition 4.20: *Let Γ_2 be a sublattice of $\Gamma_1 \subseteq \mathbb{R}^d$, $\{0 = c_0, c_1, \ldots, c_{m-1}\}$ be a complete set of coset representatives of Γ_2 in Γ_1, and $R \in OC(\Gamma_1)$.*

(i) *$R \in \mathcal{E}$ if and only if $|\sigma| = m$, where $\sigma = \{(c_j, c_k) : Rc_j - c_k \in \Gamma_2 + R\Gamma_2\}$.*
(ii) *$R \in \mathcal{H}$ if and only if none of c_j and Rc_j, $1 \le j \le m-1$, are in $\Gamma_2 + R\Gamma_2$.*
(iii) *If $c_j + \Gamma_2 \in \langle c_k + \Gamma_2 \rangle$, then $OC(c_k + \Gamma_2) \subseteq OC(c_j + \Gamma_2)$. In particular, if $\langle c_j + \Gamma_2 \rangle = \langle c_k + \Gamma_2 \rangle$, then $OC(c_j + \Gamma_2) = OC(c_k + \Gamma_2)$.*

Proof:

(i) This is immediate from Theorem 4.17(ii).
(ii) It follows from Theorem 2.8 and Lemma 2.2 that $R \in \mathcal{H}$ if and only if $\Gamma_2 \cap \Gamma_1(R) = R\Gamma_2 \cap \Gamma_1(R) = \Gamma_2(R)$. The latter is satisfied if and only if $M = N = \{c_0 + \Gamma_2 = \Gamma_2\}$ by Theorem 4.17(i). This proves the claim.
(iii) If $c_j + \Gamma_2 \in \langle c_k + \Gamma_2 \rangle$, then $c_j = nc_k + \ell$ for some $n \in \mathbb{N}$ and $\ell \in \Gamma_2$. Take an $R \in OC(c_k + \Gamma_2)$. Then $Rc_k - c_k \in \Gamma_2 + R\Gamma_2$ by Theorem 3.8. This implies that $R \in OC(c_j + \Gamma_2)$ because $Rc_j - c_j = n(Rc_k - c_k) + R\ell - \ell \in \Gamma_2 + R\Gamma_2$.

■

Results in this subsection allow the following detailed description of the case when the index of the sublattice Γ_2 in Γ_1 is prime (compare with Proposition 2.15).

Proposition 4.21: *Let $\Gamma_1 \subseteq \mathbb{R}^d$ be a lattice, Γ_2 be a sublattice of Γ_1 of index prime p, $\{0 = c_0, c_1, \ldots, c_{p-1}\}$ be a complete set of coset representatives of Γ_2 in Γ_1, and $R \in OC(\Gamma_1)$. Then exactly one of the following holds:*

(i) *If $u = 1$ and $t = p$, then $\Sigma_1(R) = \Sigma_2(R)$ and $\Gamma_1(R) = \bigcup_{k=0}^{p-1} \left[\tilde{\tilde{c}}_k + \Gamma_2(R)\right]$, where for each $0 \le k \le p-1$, $\tilde{\tilde{c}}_k = c_k + \ell_{j,k}$ with $Rc_j - c_k \in \ell_{j,k} + R\Gamma_2$ for some c_j, $0 \le j \le p-1$, and $\ell_{j,k} \in \Gamma_2$. In addition, $R \in \mathcal{H}$ if and only if $v = 1$.*
(ii) *If $u = p$ and $t = 1$, then $\Sigma_1(R) = \Sigma_2(R)$ and $\Gamma_1(R) = \bigcup_{j=0}^{p-1} [\ell_j + \Gamma_2(R)]$ where $\ell_j \in \Gamma_2$ and $Rc_j \in \ell_j + R\Gamma_2$ for each j, $0 \le j \le p-1$. Also, $R \notin \mathcal{H}$.*
(iii) *If $u = t = 1$, then $R \in \mathcal{H}$, $\Sigma_1(R) = p\,\Sigma_1(R)$, and $\Gamma_1(R) = \Gamma_2(R)$.*
(iv) *If $u = t = p$, then $\Sigma_1(R) = \frac{1}{p}\Sigma_2(R)$ and $R \notin \mathcal{H}$. Let $Rc_j \in \ell_j + R\Gamma_2$ with $\ell_j \in \Gamma_2$ for each j, $0 \le j \le p-1$, and for each k, $0 \le k \le p-1$, take $\tilde{\tilde{c}}_k = c_k + \ell_{j,k}$ with $Rc_j - c_k \in \ell_{j,k} + R\Gamma_2$ for some c_j, $0 \le j \le p-1$, and $\ell_{j,k} \in \Gamma_2$. Then*

$$\Gamma_1(R) = \bigcup_{k=0}^{p-1} \left[\tilde{\tilde{c}}_k + \left(\bigcup_{j=0}^{p-1} [\ell_j + \Gamma_2(R)]\right)\right].$$

Furthermore, $OC(c_j + \Gamma_2) = OC(c_k + \Gamma_2)$ *for all* j, k *with* $1 \le j, k \le p - 1$.

Proof: The divisibility conditions $t \mid p$, $s \mid p$, and $u \mid s$ from Theorem 4.17(ii) justify the four possible conditions set forth above. One obtains $M = \{\Gamma_2\}$, $M = \Gamma_1/\Gamma_2$, $K = \{\Gamma_2\}$, and $K = \Gamma_1/\Gamma_2$ when $u = 1$, $u = p$, $t = 1$, and $t = p$, respectively, by Theorem 4.17(i). Applying Theorems 4.17(ii) and (iii), (4.12), and Theorem 2.8 with Lemma 2.2 yields (i)–(iv).

Since Γ_1/Γ_2 is an abelian group of order prime p, $\Gamma_1/\Gamma_2 \cong \mathbb{Z}_p$. This means that $\langle c_j + \Gamma_2\rangle = \langle c_k + \Gamma_2\rangle$ for each j, k with $1 \le j, k \le p - 1$. Thus, $OC(c_j + \Gamma_2) = OC(c_k + \Gamma_2)$ by Proposition 4.20(iii). ∎

4.3. Some examples

We end this thesis by looking at several examples that make use of the results from Subsection 4.2.2.

4.3.1. Primitive rectangular lattices. Identify the square lattice Γ_2 with $\mathbb{Z}[i]$ and the $m \times 1$–primitive rectangular lattice Γ_1 with the lattice generated by $\frac{1}{m}$ and i in the complex plane, that is, $\Gamma_1 = \langle \frac{1}{m}, i\rangle_{\mathbb{Z}}$ with $m \in \mathbb{N} \setminus \{1\}$, . Then Γ_2 is a sublattice of Γ_1 of index m. Write $\Gamma_1 = \bigcup_{j=0}^{m-1} (c_j + \Gamma_2)$ where $c_j := \frac{j}{m}$ for $0 \le j \le m - 1$. Let $R = R_{z,\varepsilon} \in SOC(\Gamma_1)$, where $R_{z,\varepsilon}$ corresponds to multiplication by the complex number $\varepsilon \frac{z}{\overline{z}}$ (see Remark 1.11).

Theorem 4.17 suggests that one should start by computing for the values of $u = |M|$ and $v = |N|$ (refer to (4.11)). Now, it follows from Remark 3.25(i) that t does not divide εz and $\overline{z}$ whenever $t \in \mathbb{N} \setminus \{1\}$. This implies that $\overline{z}\frac{j}{m}, \varepsilon z\frac{j}{m} \notin \mathbb{Z}[i]$ for $1 \le j \le m-1$. Consequently, $c_j, Rc_j \notin \frac{1}{\overline{z}}\mathbb{Z}[i] = \Gamma_2 + R\Gamma_2$, and hence, $M = N = \{\Gamma_2\}$. Thus, $u = v = 1$.

Let $T = R_{z,\varepsilon} \cdot T_r \in OC(\Gamma_1)$. Then $\Gamma_2 + T\Gamma_2 = \Gamma_2 + R\Gamma_2$ and $Tc_j = Rc_j$ for each j, $0 \le j \le m - 1$. The results above then also hold for T.

Therefore, by Theorem 2.8 and Lemma 2.2, all coincidence isometries of Γ_1 are color coincidences of the coloring of Γ_1 induced by Γ_2. That is, $\mathcal{H} = OC(\Gamma_1)$. Moreover, for all $R \in OC(\Gamma_1)$, $\Sigma_1(R) = \frac{m}{t}\Sigma_2(R)$ where $t \mid m$ by Theorem 4.17(ii).

For the rest of the subsection, take m to be an odd rational prime p. Then, $t \in \{1, p\}$, and so $\Sigma_1(R) \in \{\Sigma_2(R), p\,\Sigma_2(R)\}$ for all $R \in OC(\Gamma_1)$.

It follows from Proposition 4.21 (also from Lemma 3.28 together with Proposition 3.23(i)) that $OC(c_1 + \Gamma_2) = \cdots = OC(c_{p-1} + \Gamma_2)$. Thus, if $R \in OC(c_1 + \Gamma_2)$ then $Rc_j - c_j \in \Gamma_2 + R\Gamma_2$ for all $0 \le j \le p - 1$ by Theorem 3.8. Hence, in this instance, $t = s = p$ by Theorem 4.17(i), and so $\Sigma_1(R) = \Sigma_2(R)$. Furthermore, it follows from Proposition 4.19 that R fixes all colors in the coloring of Γ_1.

Take $R = R_{z,\varepsilon} \in SOC(\Gamma_1)$. For $1 \le j \le p - 1$,

$$Rc_j - c_1 \in \Gamma_2 + R\Gamma_2 \iff \varepsilon\frac{z}{\overline{z}}\frac{j}{p} - \frac{1}{p} \in \frac{1}{\overline{z}}\mathbb{Z}[i] \iff p \mid (\varepsilon jz - \overline{z}). \tag{4.15}$$

One has

$$\varepsilon jz-\overline{z}=\begin{cases}(j-1)\mathrm{Re}\,(z)+(j+1)\mathrm{Im}\,(z)\,i, & \text{if } \varepsilon=1\\ -(j+1)\mathrm{Re}\,(z)-(j-1)\mathrm{Im}\,(z)\,i, & \text{if } \varepsilon=-1\\ -[\mathrm{Re}\,(z)+j\mathrm{Im}\,(z)]+[j\mathrm{Re}\,(z)+\mathrm{Im}\,(z)]i, & \text{if } \varepsilon=i\\ [-\mathrm{Re}\,(z)+j\mathrm{Im}\,(z)]+[-j\mathrm{Re}\,(z)+\mathrm{Im}\,(z)]i, & \text{if } \varepsilon=-i.\end{cases}$$

Since $\mathrm{Re}\,(z)$ and $\mathrm{Im}\,(z)$ are relatively prime (see Remark 3.25(i)), $p\nmid(\varepsilon jz-\overline{z})$ for each ε whenever $2\leq j\leq p-2$.

Let $k=p-1$. Observe that $p\mid[\varepsilon(p-1)z-\overline{z}]$ if and only if $p\mid(-\varepsilon z-\overline{z}\,)$. This means that $Rc_{p-1}-c_1\in\Gamma_2+R\Gamma_2$ if and only if $R_{z,-\varepsilon}c_1-c_1\in\Gamma_2+R_{z,-\varepsilon}\Gamma_2$. Hence, by Theorem 3.8, if $R_{z,-\varepsilon}\in SOC(c_1+\Gamma_2)$ then $t>1$ by Theorem 4.17(i). Since $t\in\{1,p\}$, $t=s=p$ and $\Sigma_1(R)=\Sigma_2(R)$.

Altogether, for all $R=R_{z,\varepsilon}\in SOC(\Gamma_1)$, $t=p$ if and only if $R\in SOC(c_1+\Gamma_2)$ or $R_{z,-\varepsilon}\in SOC(c_1+\Gamma_2)$. Note that at most one of the latter two conditions can be true because of Proposition 3.33(i).

These results also hold for $T_{z,\varepsilon}\in OC(\Gamma_1)\setminus SOC(\Gamma_1)$. The above calculations, together with Proposition 4.19 and Theorem 4.17(iii), yield the following theorem.

Theorem 4.22: *Let $m\in\mathbb{N}\setminus\{1\}$ and Γ be the $m\times 1$–primitive rectangular lattice viewed as the lattice $\Gamma=\langle\frac{1}{m},i\rangle_{\mathbb{Z}}$ in the complex plane. Consider the coloring of Γ determined by its square sublattice $\mathbb{Z}[i]$.*

(i) *Then $\mathcal{H}=OC(\Gamma)=OC(\mathbb{Z}[i])$ and $\Sigma_{\mathbb{Z}[i]}(R)\mid\Sigma_\Gamma(R)$ for all $R\in OC(\Gamma)$.*

(ii) *Suppose that m is an odd rational prime p and $R=R_{z,\varepsilon}\in SOC(\Gamma)$. Set $c_j=\frac{j}{p}$, for $0\leq j\leq p-1$, so that the coloring of Γ has colors $c_0,\ldots,c_{p-1}$.*

(a) *If R or $R_{z,-\varepsilon}\in SOC(c_1+\mathbb{Z}[i])$ then $\Sigma_\Gamma(R)=N(z)=z\cdot\overline{z}$. In addition,*

(i) *if $R\in SOC(c_1+\mathbb{Z}[i])$ where $Rc_1-c_1\in\ell+R\mathbb{Z}[i]$ with $\ell\in\mathbb{Z}[i]$, then $\Gamma(R)=\bigcup\limits_{k=0}^{p-1}\left[\tilde{\tilde{c}}_k+(z)\right]$, where $\tilde{\tilde{c}}_k=c_k+k\ell$. Also, R fixes all colors.*

(ii) *if $R_{z,-\varepsilon}\in SOC(c_1+\mathbb{Z}[i])$ where $Rc_{p-1}-c_1\in\ell+R\mathbb{Z}[i]$ with $\ell\in\mathbb{Z}[i]$, then $\Gamma(R)=\bigcup\limits_{k=0}^{p-1}\left[\tilde{\tilde{c}}_k+(z)\right]$, where $\tilde{\tilde{c}}_k=c_k+k\ell$. Also, R induces the permutation $(c_1\ c_{p-1})(c_2\ c_{p-2})\ldots\left(c_{\frac{p-1}{2}}\ c_{\frac{p+1}{2}}\right)$ of colors.*

(b) *Otherwise, $\Sigma_\Gamma(R)=p\,N(z)$, $\Gamma(R)=(z)$, and R is a (trivial) color coincidence, that is, R fixes the only color c_0.*

Let $T=R\cdot T_r\in OC(\Gamma)$. Then T satisfies the same properties as its rotation part R.

Example 4.23: Let Γ be a 3×1– primitive rectangular lattice. Identify Γ with the lattice $\langle\frac{1}{3},i\rangle_{\mathbb{Z}}$ in the complex plane. Recall from Example 3.39 that $OC(\frac{1}{3}+\mathbb{Z}[i])=SOC(\frac{1}{3}+\mathbb{Z}[i])\rtimes\langle T_r\rangle$, where $SOC(\frac{1}{3}+\mathbb{Z}[i])\cong\mathbb{Z}^{(\aleph_0)}$. This is because for each possible numerator z, a unique unit ε of $\mathbb{Z}[i]$ exists so that $R_{z,\varepsilon}\in SOC(\frac{1}{3}+\mathbb{Z}[i])$. Theorem 4.22, together with this result, solves the coincidence problem for Γ.

Let $f_\Gamma(m)$ and $\hat{f}_\Gamma(m)$ be the number of CSLs and coincidence rotations of Γ of index m, respectively. Then $\hat{f}_\Gamma(m) = 2f_\Gamma(m)$, where $f_\Gamma(m)$ is multiplicative with

$$f_\Gamma(p^r) = \begin{cases} 2, & \text{if } p \equiv 1 \pmod 4 \\ 1, & \text{if } p^r = 3 \\ 0, & \text{otherwise,} \end{cases}$$

for primes p and $r \in \mathbb{N}$. The Dirichlet series generating function for $f_\Gamma(m)$ is given by (see (1.3))

$$\begin{aligned} \Phi_\Gamma(s) &= \sum_{m=1}^{\infty} \frac{f_\Gamma(m)}{m^s} = (1 + 3^{-s}) \cdot \Phi_{\mathbb{Z}^2}(s) \\ &= 1 + \tfrac{1}{3^s} + \tfrac{2}{5^s} + \tfrac{2}{13^s} + \tfrac{2}{15^s} + \tfrac{2}{17^s} + \tfrac{2}{25^s} + \tfrac{2}{29^s} + \tfrac{2}{37^s} + \tfrac{2}{39^s} + \tfrac{2}{41^s} + \tfrac{2}{51^s} + \tfrac{2}{53^s} + \tfrac{2}{61^s} \\ &\quad + \tfrac{4}{65^s} + \tfrac{2}{73^s} + \cdots . \end{aligned}$$

4.3.2. Certain centered rectangular lattices. Let $\Gamma_2 = \mathbb{Z}[i]$. Consider the lattice $\Gamma_1 = \left\langle 1, \frac{1}{m}(1+i) \right\rangle_{\mathbb{Z}}$ in the complex plane, where $m \in \mathbb{N} \setminus \{1\}$. Then Γ_2 is a sublattice of Γ_1 of index m. Let $c_j := \frac{j}{m}(1+i)$ for $0 \le j \le m-1$ so that $\{c_0, \ldots, c_{m-1}\}$ is a complete set of coset representatives of Γ_2 in Γ_1. Take $R = R_{z,\varepsilon} \in SOC(\Gamma_1)$.

If $t \in \mathbb{N} \setminus \{1\}$ then $t \nmid \overline{z}(1+i)$ and $t \nmid \varepsilon z(1+i)$ by Remark 3.25(i). Hence, $\overline{z}\frac{j}{m}(1+i), \varepsilon z \frac{j}{m}(1+i) \notin \mathbb{Z}[i]$, for $1 \le j \le m-1$. This implies that $c_j, Rc_j \notin \Gamma_2 + R\Gamma_2$, and thus, $u = v = 1$ by Theorem 4.17(i).

Let $T = T_{z,\varepsilon} \in OC(\Gamma_1) \setminus SOC(\Gamma_1)$. If one writes T as $T = R_{z,-i\varepsilon} T_{1,i}$, then $\Gamma_2 + T\Gamma_2 = \Gamma_2 + R_{z,-i\varepsilon}\Gamma_2$ and $Tc_j = R_{z,-i\varepsilon} c_j$ for $0 \le j \le m-1$. This means that the results above are also true for T.

It follows from Theorem 2.8 and Lemma 2.2 that $\mathcal{H} = OC(\Gamma_1)$, that is, all coincidence isometries of Γ_1 are color coincidences of the coloring of Γ_1 determined by Γ_2. In addition, for all $R \in OC(\Gamma_1)$, $\Sigma_1(R) = \frac{m}{t}\Sigma_1(R)$, where $t \mid m$, by Theorem 4.17(ii).

From this point until the end of the subsection, assume that m is an odd prime p. In such a case, Γ_1 is a centered rectangular lattice. Here, $t \in \{1, p\}$ which implies that $\Sigma_1(R) \in \{\Sigma_2(R), p\,\Sigma_2(R)\}$ for all $R \in OC(\Gamma_1)$.

Note that $OC(c_1 + \Gamma_2) = \cdots = OC(c_{p-1} + \Gamma_2)$ by Proposition 4.21 (or by Lemma 3.28 and Proposition 3.23(i)). It follows then from Theorem 3.8 that if $R \in OC(c_1 + \Gamma_2)$ then $Rc_j - c_j \in \Gamma_2 + R\Gamma_2$ for all $0 \le j \le p-1$. Thus, by Theorem 4.17(i), $t = s = p$ and so $\Sigma_1(R) = \Sigma_2(R)$ for all such R. Also, R fixes all the colors in the coloring of Γ_1 by Proposition 4.19.

Let $R = R_{z,\varepsilon} \in SOC(\Gamma_1)$. Keep in mind that $t \in \{1, p\}$. For $1 \le j \le p-1$,

$$Rc_j - c_1 \in \Gamma_2 + R\Gamma_2 \iff \varepsilon \tfrac{z}{\overline{z}} \tfrac{j(1+i)}{p} - \tfrac{1+i}{p} \in \tfrac{1}{\overline{z}}\mathbb{Z}[i] \iff \tfrac{(1+i)(\varepsilon j z - \overline{z})}{p} \in \mathbb{Z}[i] \iff p \mid (\varepsilon j z - \overline{z}),$$

since p is relatively prime to $1+i$. Observe that what we have here is exactly the same condition as in (4.15), wherein we were looking at the coincidences of the $p \times 1$–primitive rectangular lattice. Thus, results obtained from the previous subsection must still hold.

Given $T = T_{z,\varepsilon} = R_{z,-i\varepsilon}T_{1,i} \in OC(\Gamma_1)$, one has $Tc_j - c_1 \in \Gamma_2 + T\Gamma_2$ if and only if $R_{z,-i\varepsilon}c_j - c_1 \in \Gamma_2 + R_{z,-i\varepsilon}\Gamma_2$. This means that the results for $T_{z,\varepsilon}$ are the same as that of the corresponding rotation $R_{z,-i\varepsilon}$.

All these information yield the next theorem. The CSL $\Gamma(R)$ and the color permutation that the color coincidence R effects were computed using Theorem 4.17(iii) and Proposition 4.19, respectively.

Theorem 4.24: *Let $m \in \mathbb{N} \setminus \{1\}$ and Γ be the lattice with basis $\left\{1, \frac{1}{m}(1+i)\right\}$ in the complex plane. Consider the coloring of Γ induced by the square sublattice $\mathbb{Z}[i]$ of Γ.*

(i) *Then $\mathcal{H} = OC(\Gamma) = OC(\mathbb{Z}[i])$ and $\Sigma_{\mathbb{Z}[i]}(R) \mid \Sigma_\Gamma(R)$ for all $R \in OC(\Gamma)$.*

(ii) *Suppose m is an odd rational prime p and $R = R_{z,\varepsilon} \in SOC(\Gamma)$. Take $c_j = \frac{j}{p}(1+i)$, for $0 \le j \le p-1$, so that the coloring of Γ consists of the colors $c_0, \ldots, c_{p-1}$.*

  (a) *If R or $R_{z,-\varepsilon} \in SOC(c_1 + \mathbb{Z}[i])$ then $\Sigma_\Gamma(R) = N(z)$. In addition,*

    (i) *if $R \in SOC(c_1 + \mathbb{Z}[i])$ where $Rc_1 - c_1 \in \ell + R\mathbb{Z}[i]$ with $\ell \in \mathbb{Z}[i]$, then $\Gamma(R) = \bigcup_{k=0}^{p-1}\left[\tilde{\tilde{c}}_k + (z)\right]$, where $\tilde{\tilde{c}}_k = c_k + k\ell$. Also, R fixes all colors.*

    (ii) *if $R_{z,-\varepsilon} \in SOC(c_1 + \mathbb{Z}[i])$ where $Rc_{p-1} - c_1 \in \ell + R\mathbb{Z}[i]$ with $\ell \in \mathbb{Z}[i]$, then $\Gamma(R) = \bigcup_{k=0}^{p-1}\left[\tilde{\tilde{c}}_k + (z)\right]$, where $\tilde{\tilde{c}}_k = c_k + k\ell$. Also, R effects the permutation $(c_1\ c_{p-1})(c_2\ c_{p-2})\ldots\left(c_{\frac{p-1}{2}}\ c_{\frac{p+1}{2}}\right)$ of colors.*

  (b) *Otherwise, $\Sigma_\Gamma(R) = p\,N(z)$, $\Gamma(R) = (z)$, and R fixes the only color c_0.*

Let $T_{z,\varepsilon} \in OC(\Gamma) \setminus SOC(\Gamma)$. Then $T_{z,\varepsilon}$ has exactly the same properties as the rotation $R_{z,-i\varepsilon}$.

The following corollary follows directly from Theorems 4.22, 4.24, and 1.3.

Corollary 4.25: *Let Γ_P and Γ_C be $p \times 1$–primitive and centered rectangular lattices, respectively, where p is an odd prime. If $f_{\Gamma_P}(m)$ and $f_{\Gamma_C}(m)$ count the number of CSLs of Γ_P and Γ_C of index m, respectively, then $f_{\Gamma_P}(m) = f_{\Gamma_C}(m)$ for all $m \in \mathbb{N}$.*

EXAMPLE 4.26: Let Γ be the centered rectangular lattice $\left\langle 1, \frac{1}{5}(1+i)\right\rangle_{\mathbb{Z}}$ in the complex plane. In Example 3.41, it was shown that $OC(\frac{1+i}{5} + \mathbb{Z}[i]) = SOC(\frac{1}{5} + \mathbb{Z}[i]) \rtimes \langle T_{1,i}\rangle$, where $SOC(\frac{1}{5} + \mathbb{Z}[i]) \cong \mathbb{Z}^{(\aleph_0)}$ because for each possible numerator z with $5 \nmid N(z)$, there exists a unique unit ε of $\mathbb{Z}[i]$ such that $R_{z,\varepsilon} \in SOC(\frac{1}{5} + \mathbb{Z}[i])$. With this result, Theorem 4.24 can be applied to solve the coincidence problem for Γ.

Denote by $f_\Gamma(m)$ and $\hat{f}_\Gamma(m)$ the number of CSLs and coincidence rotations of Γ for a given index m, respectively. Then

$$\hat{f}_\Gamma(m) = \begin{cases} 2f_\Gamma(m), & \text{if } 25 \nmid m \\ 4f_\Gamma(m), & \text{if } 25 \mid m. \end{cases}$$

Also, $f_\Gamma(m)$ is multiplicative, and for primes p and $r \in \mathbb{N}$,

$$f_\Gamma(p^r) = \begin{cases} 2, & \text{if } p \equiv 1 \pmod 4 \text{ and } p^r \neq 5 \\ 1, & \text{if } p^r = 5 \\ 0, & \text{otherwise.} \end{cases}$$

The Dirichlet series generating function for $f_\Gamma(m)$ is given by

$$\Phi_\Gamma(s) = \sum_{m=1}^{\infty} \frac{f_\Gamma(m)}{m^s} = \frac{1+5^{-2s}}{1-5^{-s}} \prod_{\substack{p\equiv 1(4)\\ p\neq 5}} \frac{1+p^{-s}}{1-p^{-s}}$$
$$= 1 + \tfrac{1}{5^s} + \tfrac{2}{13^s} + \tfrac{2}{17^s} + \tfrac{2}{25^s} + \tfrac{2}{29^s} + \tfrac{2}{37^s} + \tfrac{2}{41^s} + \tfrac{2}{53^s} + \tfrac{2}{61^s} + \tfrac{2}{65^s} + \tfrac{2}{73^s} + \cdots.$$

4.3.3. Other examples. Theorem 4.22 gives the complete solution of the coincidence problem for an $m \times 1$–primitive rectangular lattice only if m is an odd prime. The following example examines the case when $m = 4$.

Example 4.27: Consider the 4×1–primitive rectangular lattice identified with the lattice $\Gamma_1 = \langle \frac{1}{4}, i\rangle_{\mathbb{Z}}$ in the complex plane. Then $\Gamma_2 = \mathbb{Z}[i]$ is a sublattice of Γ_1 of index 4. Let $c_j := \frac{j}{4}$ for $0 \leq j \leq 3$, so that $\Gamma_1 = \bigcup_{j=0}^{3} (c_j + \Gamma_2)$. Consider the coloring of Γ_1 determined by Γ_2 with colors c_0, c_1, c_2, and c_3.

Theorem 4.22 indicates that $\mathcal{H} = OC(\Gamma_1) = OC(\Gamma_2)$. Since $t \mid 4$, $t \in \{1,2,4\}$, and so $\Sigma_1(R) \in \{\Sigma_2(R), 2\Sigma_2(R), 4\Sigma_2(R)\}$. Recall from Examples 3.40 and 3.38 that

$$OC(c_1+\Gamma_2) = OC(c_3+\Gamma_2) = \left\{R_{z,\varepsilon} \in SOC(\Gamma_2) : \varepsilon = (-1)^{\mathrm{Im}(z)}\right\} \rtimes \langle T_r\rangle$$

and $OC(c_2+\Gamma_2) = \{R_{z,\varepsilon} \in SOC(\Gamma_2) : \varepsilon = \pm 1\}$.

Since $OC(c_1+\Gamma_2) \subseteq OC(c_2+\Gamma_2)$, $Rc_j - c_j \in \Gamma_2 + R\Gamma_2$ for $0 \leq j \leq 3$ whenever $R \in OC(c_1+\Gamma_2)$ by Theorem 3.8. Here, $t = s = 4$ by Theorem 4.17(i) and thus, $\Sigma_1(R) = \Sigma_2(R)$. Furthermore, R fixes all colors in the coloring of Γ_1 by Proposition 4.19.

Before proceeding, note that if $j,k \in \mathbb{N}$ then

$$\varepsilon jz - k\overline{z} = \begin{cases} (j-k)\mathrm{Re}\,(z) + (j+k)\mathrm{Im}\,(z)\,i, & \varepsilon = 1 \\ -(j+k)\mathrm{Re}\,(z) - (j-k)\mathrm{Im}\,(z)\,i, & \varepsilon = -1 \\ -[j\mathrm{Im}\,(z) + k\mathrm{Re}\,(z)] + [j\mathrm{Re}\,(z) + k\mathrm{Im}\,(z)]i, & \varepsilon = i \\ [j\mathrm{Im}\,(z) - k\mathrm{Re}\,(z)] + [-j\mathrm{Re}\,(z) + k\mathrm{Im}\,(z)]i, & \varepsilon = -i. \end{cases} \tag{4.16}$$

Let $R = R_{z,\varepsilon} \in SOC(c_2+\Gamma_2) \setminus SOC(c_1+\Gamma_2)$, that is, $\varepsilon = (-1)^{\mathrm{Re}(z)}$. In this instance, $Rc_j - c_j \in \Gamma_2 + R\Gamma_2$ if and only if $j \in \{0,2\}$ by Theorem 3.8. It follows then from Theorem 4.17(i) that $s = t = 4$ if $Rc_3 - c_1 \in \Gamma_2 + R\Gamma_2$, and $s = t = 2$ otherwise.

By (4.16),

$$\frac{(-1)^{\mathrm{Re}(z)}3z - \overline{z}}{4} = \begin{cases} \frac{1}{2}\mathrm{Re}\,(z) + \mathrm{Im}\,(z)\,i, & \text{if } \mathrm{Re}\,(z) \text{ is even} \\ -\mathrm{Re}\,(z) - \frac{1}{2}\mathrm{Im}\,(z)\,i, & \text{if } \mathrm{Im}\,(z) \text{ is even.} \end{cases}$$

Hence, $\frac{(-1)^{\mathrm{Re}(z)}3z-\overline{z}}{4} \in \mathbb{Z}[i]$, or equivalently, $Rc_3 - c_1 \in \Gamma_2 + R\Gamma_2$. Therefore, $\Sigma_1(R) = \Sigma_2(R)$. Also, by Proposition 4.19, R fixes both colors c_0 and c_2, and interchanges the colors c_1 and c_3, in the coloring of Γ_1.

The only remaining case is when $R = R_{z,\varepsilon} \in SOC(\Gamma_2) \setminus SOC(c_2 + \Gamma_2)$, that is, when $\varepsilon = \pm i$. Suppose first that $\varepsilon = i$, and consider the following possibilities:

`Case I:` $j, k \in \{1, 3\}$ with $j \neq k$

By (4.16) and Remark 3.25(i),

$$\begin{aligned}\mathrm{Re}\,(\varepsilon jz - k\overline{z}) \cdot \mathrm{Im}\,(\varepsilon jz - k\overline{z}) &= -\big[\mathrm{Re}\,(z)^2 + \mathrm{Im}\,(z)^2\big]jk - \mathrm{Re}\,(z)\,\mathrm{Im}\,(z)\,(j^2 + k^2)\\ &\equiv \big[\mathrm{Re}\,(z)^2 + \mathrm{Im}\,(z)^2\big] \pmod 4 \equiv 1 \pmod 4.\end{aligned}$$

This implies that $4 \nmid (\varepsilon jz - k\overline{z})$, and equivalently, $Rc_j - c_k \notin \Gamma_2 + R\Gamma_2$.

`Case II:` $j, k \in \{1, 2, 3\}$ with $j \neq k$ and $j \cdot k$ even

It follows from (4.16) that

$$\mathrm{Re}\,(\varepsilon jz - k\overline{z}) + \mathrm{Im}\,(\varepsilon jz - k\overline{z}) = [\mathrm{Re}\,(z) - \mathrm{Im}\,(z)](j - k) \equiv 1 \pmod 2.$$

Again, $4 \nmid (\varepsilon jz - k\overline{z})$, and equivalently, $Rc_j - c_k \notin \Gamma_2 + R\Gamma_2$.

Hence, $s = t = 1$ by Theorem 4.17(i) and $\Sigma_1(R) = 4\Sigma_2(R)$. Also, R fixes the only color c_0. Analogous arguments yield the same result for $\varepsilon = -i$.

The same results are true for coincidence reflections $T = R \cdot T_r$, where $R = R_{z,\varepsilon} \in SOC(\Gamma_1)$. This is because $T\Gamma_2 = R\Gamma_2$ and $Tc_j = Rc_j$ for $0 \leq j \leq 3$. The following proposition summarizes these results.

Proposition 4.28: *Let Γ be the 4×1–primitive rectangular lattice with basis $\left\{\frac{1}{4}, i\right\}$ in the complex plane. Suppose $R = R_{z,\varepsilon} \in SOC(\Gamma) = SOC(\mathbb{Z}[i])$. Take $c_j = \frac{j}{4}$, for $0 \leq j \leq 3$, so that the coloring of Γ determined by $\mathbb{Z}[i]$ has colors c_0, c_1, c_2, c_3.*

- (i) *If $\varepsilon = \pm 1$ then $\Sigma_\Gamma(R) = N(z)$. In addition,*
  - (a) *if $\varepsilon = (-1)^{\mathrm{Im}(z)}$ where $Rc_1 - c_1 \in \ell + R\mathbb{Z}[i]$ with $\ell \in \mathbb{Z}[i]$, then $\Gamma(R) = \bigcup_{k=0}^{3} \big[\tilde{\tilde{c}}_k + (z)\big]$, where $\tilde{\tilde{c}}_k = c_k + k\ell$. Also, R fixes all colors.*
  - (b) *if $\varepsilon = (-1)^{\mathrm{Re}(z)}$ where $Rc_2 - c_2 \in \ell_1 + R\mathbb{Z}[i]$, $Rc_3 - c_1 \in \ell_2 + R\mathbb{Z}[i]$, with $\ell_1, \ell_2 \in \mathbb{Z}[i]$, then*
  $$\Gamma(R) = (z) \cup [c_1 + \ell_2 + (z)] \cup [c_2 + \ell_1 + (z)] \cup [c_3 + 3\ell_2 + (z)].$$
  Also, R induces the permutation $(c_1\ c_3)$ of colors.
- (ii) *If $\varepsilon = \pm i$ then $\Sigma_\Gamma(R) = 4N(z)$, $\Gamma(R) = (z)$, and R is a (trivial) color coincidence, that is, R fixes the only color c_0.*

If $T = R \cdot T_r \in OC(\Gamma)$, then T has exactly the same properties as its rotation part R.

Let $f_\Gamma(m)$ and $\hat{f}_\Gamma(m)$ denote the number of CSLs and coincidence rotations of Γ of index m, respectively. Then $\hat{f}_\Gamma(m) = 2f_\Gamma(m)$, and $f_\Gamma(m)$ is multiplicative given by

$$f_\Gamma(p^r) = \begin{cases} 2, & \text{if } p \equiv 1 \pmod 4\\ 1, & \text{if } p^r = 4\\ 0, & \text{otherwise,}\end{cases}$$

for primes p and $r \in \mathbb{N}$. The Dirichlet series generating function for $f_\Gamma(m)$ reads (see (1.3)*)*

$$\begin{aligned}\Phi_\Gamma(s) = \sum_{m=1}^{\infty} \frac{f_\Gamma(m)}{m^s} &= (1+4^{-s}) \cdot \Phi_{\mathbb{Z}^2}(s) \\ &= 1 + \tfrac{1}{4^s} + \tfrac{2}{5^s} + \tfrac{2}{13^s} + \tfrac{2}{17^s} + \tfrac{2}{20^s} + \tfrac{2}{25^s} + \tfrac{2}{29^s} + \tfrac{2}{37^s} + \tfrac{2}{41^s} + \tfrac{2}{52^s} + \tfrac{2}{53^s} + \tfrac{2}{61^s} + \tfrac{4}{65^s} \\ &\quad + \tfrac{2}{68^s} + \tfrac{2}{73^s} + \cdots .\end{aligned}$$

The next example illustrates how Proposition 4.19 provides an alternative method of calculating the set of coincidence isometries of a shifted lattice.

EXAMPLE 4.29: Let $\Gamma_1 = \mathrm{Im}\,(\mathbb{L})$ and $\Gamma_2 = 2\mathrm{Im}\,(\mathbb{J})$. Then Γ_1 is a primitive cubic lattice and Γ_2 is a body-centered cubic lattice contained in Γ_1 of index 4. Write $\Gamma_1 = \bigcup_{j=0}^{3} (c_j + \Gamma_2)$ where $c_0 = 0$, $c_1 = \mathbf{i}$, $c_2 = \mathbf{j}$, and $c_3 = \mathbf{k}$, and consider the coloring of Γ_1 determined by Γ_2.

It was shown in Example 2.18 that $\mathcal{H} = OC(\Gamma_1)$ and for every $R \in OC(\Gamma_1)$, $s = t = 4$. Hence, by Proposition 4.19, $OC(c_j + \Gamma_2)$ consists of all $R \in OC(\Gamma_1)$ that fix color c_j, for $j \in \{1,2,3\}$. If $r_1 = (1,1,0,0)$, $r_2 = (1,0,1,0)$, and $r_3 = (1,0,0,1)$, then one obtains from Example 2.18 that

$$OC(c_j + \Gamma_2) = \left\{ R_q \in OC(\Gamma_1) : |q|^2 \text{ is odd or } |q|^2 \equiv 2 \pmod 4 \text{ with } q \in r_j + 2\mathbb{J} \right\}.$$

It can be verified that $OC(c_j + \Gamma_2)$ is closed under composition, and hence is a group by Proposition 3.14.

Finally, suppose $f_{c_j+\Gamma_2}(m)$ and $\hat{f}_{c_j+\Gamma_2}(m)$ count the number of CSLs and coincidence rotations of $c_j + \Gamma_2$ of index m, respectively. Since $Sc_j - c_j \in \Gamma_2$ for all $S \in P(\Gamma_2) \cap OC(c_j + \Gamma_2)$ and $j \in \{1,2,3\}$, it follows from Proposition 3.9 that $\hat{f}_{c_j+\Gamma_2}(m) = 8 f_{c_j+\Gamma_2}(m)$ and $f_{c_j+\Gamma_2}(m) = f_{\mathbb{Z}^3}(m)$.

Outlook

The question of whether the set of color coincidences of a coloring of a lattice determined by some sublattice forms a group or not is yet to be resolved. A negative answer is highly suspected, and a counterexample will not only confirm this fact, but should also shed more light on the coincidence index of a product of two coincidence isometries. On the other hand, the set of affine coincidence isometries of a lattice, and the set of coincidence isometries of a shifted lattice are not groups in general. Although, an example where the set of coincidence rotations of a shifted lattice fails to form a group is still lacking. Such an example might be found in three-dimensions, where $O(d)$ is not anymore Abelian. Furthermore, it could be worthwhile to take a closer look at the algebraic structures of all these new subsets of $O(d)$ and $E(d)$.

The generalization of a color symmetry to color coincidences is not only interesting in its own right, but it also provides a further connection between the relationship of the coincidence indices of a lattice and sublattice. Moreover, Theorem 2.8 permits a simpler way of determining the color groups of colorings of lattices and $\mathbb{Z}$-modules, many of which are yet to be determined. It would also be helpful if a similar connection between similar sublattices (SSLs) and colorings of lattices can be set up. This would give a more unified perspective among SSLs, CSLs, and colorings of lattices.

From the results of this thesis, it is foreseeable that the coincidence indices of other types of lattices may be calculated, as long as the lattices can be treated as sublattices (or parent lattices) of other lattices for which the coincidence problem has already been completely solved. Most of the worked-out examples in this thesis was done for planar lattices. It should be beneficial to implement the results of this thesis to compute for the coincidence indices of various lattices and $\mathbb{Z}$-modules in higher dimensions.

The purpose of this thesis is to shed further light on the geometry of CSLs and CSMs. It would certainly be productive to explore the implications of the results in this thesis to the actual study of grain boundaries of crystals and quasicrystals.

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